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Explanatory Notes on W. H. Zachariasen's "Theory of X-Ray Diffraction in Ideal Crystals"

MOHAMMAD FATEMI

X-Ray Optics Branch
Nuclear Sciences Division

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NAVAL RESEARCH LABORATORY
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ERRATA

Page 5. Fourth equation: Change u_2 and p_2 to u_z and p_z.

Page 28. Third equation from the bottom: Insert an integral sign $\int$ in front of $\Omega_j \, dv$.

Page 29. A — Replace the statement: "which may be rewritten as..." with "subject to

$$(1 + \psi)\mathbf{E} = \varepsilon\,\mathbf{E} = \mathbf{D}$$

which may be rewritten as

$$(1 - \psi)\mathbf{D} = \mathbf{E}"$$

B — Third equation from the bottom: The subscript of β in the last exponent is L rather than H.

Page 32. Top line should read:

$$= \sum \boldsymbol{\beta}_H \cdot \mathbf{D}_H e^{i\omega_0 t - i2\pi\boldsymbol{\beta}_H \cdot \mathbf{r}} \,,$$

Page 39. Fourth equation: The first term on the right should read

$$"- 2\,\frac{1}{\lambda_0}\,\frac{1}{\lambda_B}."$$

Page 45: Last equation: Replace "$\sinh^2 \theta = ...$" with "$2 \sinh^2 \theta = ...$"

Page 54. Last equation: Correct the term "$1 - \frac{1}{y^2}$" to $\sqrt{1 - \frac{1}{y^2}}$

Page 55. A — Top equation: Correct the last term to $1 - \sqrt{1 - y^{-2}}$

B — Second equation: The upper limit of the first integral on the right is -1 rather than ∞.

Page 60. Last part of last equation should read $\dfrac{\mu_0 t_0}{\gamma_0}\,\varepsilon$.

Page 61. Second equation should read

$$\sinh^2 x = \frac{(e^x - e^{-x})^2}{4} = \frac{e^{2x} + e^{-2x} - 2}{4} \,.$$

CONTENTS

PREFACE

One aim of the X-Ray Optics Branch during the past years has been an understanding of the diffraction properties of crystals and their characterization on the basis of defect structure. For this purpose, my coworkers and I have carried out both experimental and theoretical investigations in diffraction and have compared our results with the mathematical and physical models that have been available in the works of various authors.

A reference we have believed to be a source of many subtle ideas in the diffraction field is Zachariasen's 1945 book, *Theory of X-Ray Diffraction in Crystals.* However, Zachariasen's presentation of the mathematical information is in general too brief. Thus, in contrast to his verbal description of the physical process, which is often quite lucid, many of his significant derivations have a striking absence of intermediate steps. Although no reader would like to see all the detail, we believe that the more difficult steps should be accompanied by at least a few comments that would indicate the point at which underlying mathematical approximations have been introduced.

The present set of notes on Chapter III ("Theory of X-Ray Diffraction in Ideal Crystals") of Zachariasen's book is intended to partially remove this deficiency of explanatory comments. Initially, comments were written both for Chapter III and that part of Chapter IV which precedes the section on "Heat Motion." Prior to their introduction as an NRL Report, however, the notes had to be modified somewhat. First, to make them useful to readers with diverse levels of mathematical background, considerable effort was made to give explanations and derivations of formulas in as elementary a fashion as possible. (For example the notes begin with simple illustrations of the periodic functions.) This has not always been practical, of course, and several concepts will nevertheless remain difficult. The emphasis has been on those numerous derivations which require special mathematical tools and clever steps in reasoning and approximation.

Second, as a compromise in the amount of material presented, Chapter III alone was prepared for this NRL Report. In fact, Chapter IV is much easier to understand once the concepts of Chapter III are clarified. These notes are only a supplement to the original chapter and are not an entity in themselves; a completely rewritten chapter would probably have tripled the size of this work.

With the publication of this report it is hoped that at least some of the time taken by the serious student of diffraction theory would be better spent in thinking about new solutions to old problems (such as the concept of "mosaic block"), which at the same time realizing the economy and profundity of Zachariasen's thoughts, which have become an inseparable part of his style throughout the years.

M. Fatemi

ABSTRACT

W. H. Zachariasen's well-known 1945 book "Theory of X-Ray Diffraction in Crystals" contains many significant and original ideas pertaining to diffraction theory. However, the discussions and mathematical derivations therein lack the necessary detail which could make the text useful to readers of diverse mathematical background. The purpose of these notes is to provide additional comments and intermediate derivational steps for Chapter III of this book, "Theory of X-Ray Diffraction in Ideal Crystals," whose content has often been referenced in the published literature.

PROBLEM STATUS

This is an interim report on the NRL Problem.

AUTHORIZATION

NRL Problem P04-04

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EXPLANATORY NOTES ON W. H. ZACHARIASEN'S
"THEORY OF X-RAY DIFFRACTION IN IDEAL CRYSTALS"

INTRODUCTION

The study of x-ray diffraction in crystals ultimately leads to the measurement of a few basic parameters which, in a general sense, reflect the quality of the crystals when used in applied problems such as spectral analysis of radiation sources, analysis of compounds, radiation damage, and growth and defect structure of materials. Among these parameters are the following:

● The efficiency with which x rays of a particular energy (or wavelength) are diffracted from a crystal.

● The sharpness of diffraction peaks, that is, the resolution with which reflections from a crystal may be distinguished.

The instrument capable of such measurements is the double-crystal spectrometer. Here characteristic x rays of wavelength λ are reflected by the first crystal (monochromator) according to Bragg's law $\lambda = 2d \sin \theta$, where d is the interplanar spacing of the diffracting planes, and θ is the Bragg angle. The reflected x rays then arrive onto the second crystal, which is to be analyzed for its own perfection or to be used in the analysis of radiation incident upon its surface.

To investigate the diffraction characteristics of a crystal in a double-crystal spectrometer, the monochromator is fixed and the second crystal is rotated—or rocked—in the vicinity of the Bragg angle. The response of the crystal to the incident x-ray photons, shown by a plot of intensity versus angle, is called its rocking curve.

The peak of the rocking curve, which occurs at (or very near) the Bragg angle, is a significant parameter. The ratio of the peak intensity to the incident intensity is a dimensionless quantity called the peak diffraction efficiency. The angular width of the rocking curve, which is a measure of the sharpness of diffraction, is influenced by several geometrical factors (slit size, etc.) as well as by the perfection of both crystals. In scientific communications either the full width at half maximum (FWHM) or the half breadth at half maximum (HBHM) are quoted. The area under the rocking curve (which accounts for the total number of photons diffracted) divided by the number of incident photons is known as the integrated reflection coefficient (R value) and is expressed in units of radians.

Note: The title of this report refers to Chapter III of the book *Theory of X-Ray Diffraction in Crystals*, New York, Wiley, 1945.

The point of this introduction is to emphasize the ultimate purpose of all the derivations and explanations both here and in Zachariasen's book. These should be regarded as a means toward an experimental end: in the final analysis, any diffraction theory should be tested by a physical instrument, such as the double-crystal spectrometer. This is why such a discussion appears at the end of Zachariasen's Chapter III.

Much can be learned from any theoretical exercise, but the final value of a good theory is not only to explain experimental results but to do it on a physically sound basis and with such vigor as to enable the experimenter to apply it in further predictions.

DERIVATIONS AND EXPLANATIONS

The derivations and explanations presented here will begin with the starting pages of Chapter III and be keyed by subheadings to pages or equation numbers in the sequence of appearance in the chapter.

Page 83: Concept of a Periodic Function

A typical one-dimensional periodic function is the sine function. If the periodicity is shown by the vector **a**, an arbitrary periodic function may appear as in Fig. 1.

The vector **a** defines a specific orientation in space. Since any solid is three-dimensional, it is in general necessary to specify three directions for any periodic lattice function.

Page 83: Wave Vector **k** or $\mathbf{k_0}$

The wave vector **k** or $\mathbf{k_0}$ is defined differently by various authors. In quantum mechanics the more usual notation is $k_0 = 2\pi/\lambda_0$, whereas others prefer $k = 1/\lambda$ without the factor 2π.
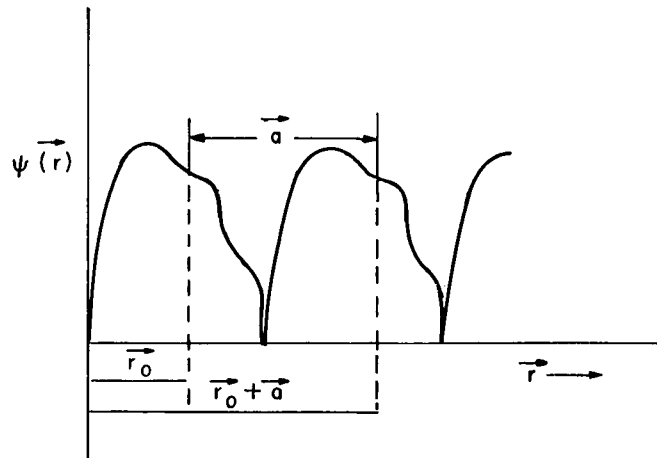
Fig. 1—An arbitrary periodic function $\Psi(\mathbf{r})$

Page 84 (and Chapter I)

A clear explanation of reciprocal lattice concepts, together with a discussion on the equivalence of Bragg's law and Laue diffraction conditions, is given by Azaroff [1].

Figure 3.2

Figure 3.2 is a diagram drawn in the reciprocal lattice space. In this space, linear dimensions have units inverse to the "real" crystal lattice space. The "reality" of the reciprocal space, however, becomes apparent upon studying the origins of the stereographic projection.

Pages 87 and 88

Four general or three "practical" experimental methods are described. Today, however, the fourth method (continuous variation of λ together with the direction of incidence) has found a significant place in diffraction studies: The curved-crystal spectrometer described by Birks [2] has been used as an invaluable tool in spectral analysis of pulsed x-rays (flash x-ray tubes, laser-induced x rays, etc.).

Page 89

In sections 3 through 7 intensity expressions are derived on the basis of kinematical theory, for the case of a single electron, a single atom (aggregate of electrons), a unit cell (basic array of atoms), and a "small" crystallite. The dynamical theory is then treated in sections 8 through 12.

Page 90: Basic Assumptions of Thomson Scattering

The first assumption of Thomson scattering is that the restoring force on the electron is negligible. Therefore, the force due to the electric field, $e\mathbf{E}$, is the net force and accelerates the electron according to Newton's second law. The second assumption is that the natural frequency of the electron is small compared to the frequency of x rays. Thus no resonance will occur between the electron and the electromagnetic field. This means that the electron scattering intensity will be an expression *independent of x-ray frequencies.* On the basis of these assumptions, equation 3.7 follows from the simple second-order differential equation

$$-e\mathbf{E}_0 e^{i\omega_0 t} = m\frac{d^2\mathbf{x}}{dt^2} \ .$$

Equation 3.8 is a "definition" from elementary electricity and magnetism theory. Equation 3.9 also defines the coefficient of $\mathbf{E}_0$ in Equation 3.8.

Page 90: Dipole Radiation, Equation 3.10

The following texts give more explicit forms for dipole radiation by writing out various components : Becker and Sauter [3], Pugh and Pugh [4], and Panofsky and Phillips (1962) [5]. The vectorial form given by equation 3.10 will be used in the following derivation.

Derivation of Equation 3.11

The vector u is the unit vector in the direction of scattering (or observation), and p_e is the electric dipole moment. The vector $u \times p_e$ appearing in equation 3.10 is a vector normal to u and p_e. Its magnitude is

$$|u||p_e| \sin \angle(u, p_e) = |u||p_e| \sin \varphi = |p_e| \sin \varphi,$$

and its direction is determined by the right-handed screw rule. Now

$$e^{i\omega_0 t} E_e = (u \times p_e) \times u e^{i\omega_0 t - i2\pi k \cdot R},$$

$$E_e = (u \times p_e) \times u e^{-i2\pi k \cdot R},$$

$$E_e^2 = |E_e|^2 = E_e \cdot E_e^* = [(u \times p_e) \times u] \cdot [(u \times p_e) \times u].$$

Note that taking complex conjugate removes $e^{-2\pi i k \cdot R}$. Again,

$$[(u \times p_e) \times u] \perp u \quad \text{and} \quad \perp (u \times p_e) \Rightarrow [(u \times p_e) \times u] \parallel p_e.$$

Now

$$|(u \times p_e) \times u| = |u \times p_e||u| \sin \angle[(u \times p_e), u] = |u \times p_e| \cdot |u|$$

because $u \perp u \times p_e$ and $\sin \angle[(u \times p_e), u] = 1$. Thus

$$|(u \times p_e) \times u|^2 = p_e^2 \sin^2 \varphi = E_0^2 \left(\frac{e^2}{m\omega_0^2}\right) \sin \varphi.$$

Since

$$\frac{I_e}{I_0} = \frac{E_e^2}{E_0^2},$$

then equation 3.11 follows.

Page 91: Derivation of Equation 3.12

The sentence introducing equation 3.12 states that the equation is obvious. However, even though equation 3.12 may be justified by visual observation, it is not *at all* obvious.

Sin φ is defined in the relation

$$|\mathbf{u}_0 \times \mathbf{p}_e| = |\mathbf{u}_0||\mathbf{p}_e| \sin \varphi = |\mathbf{p}_e| \sin \varphi,$$

or

$$\sin \varphi = \frac{|\mathbf{u} \times \mathbf{p}_e|}{|\mathbf{p}_e|}$$

and

$$\sin^2 \varphi = \frac{|\mathbf{u} \times \mathbf{p}_e||\mathbf{u} \times \mathbf{p}_e|}{|\mathbf{p}_e|^2} = \frac{(\mathbf{u} \times \mathbf{p}_e) \cdot (\mathbf{u} \times \mathbf{p}_e)}{|\mathbf{p}_e|^2}.$$

Now define $\hat{i}, \hat{j}, \hat{k}$ as the set of unit vectors along the X, Y, Z directions. We have

$$\mathbf{u} \times \mathbf{p} = (u_y\hat{j} + u_2\hat{k}) \times (p_x\hat{i} + p_2\hat{k}),$$

which becomes, since $\hat{j} \times \hat{i} = -\hat{k}, \hat{j} \times \hat{k} = \hat{i}, \hat{k} \times \hat{i} = \hat{j}$, and $\hat{k} \times \hat{k} = 0$,

$$\mathbf{u} \times \mathbf{p} = -u_y p_x\hat{k} + u_y p_z\hat{i} + u_z p_{xj}$$

with

$$u_y = |\mathbf{u}| \cos 2\theta = \cos 2\theta, \qquad u_z = \sin 2\theta,$$

$$p_x = |\mathbf{p}| \sin \psi, \qquad p_z = |\mathbf{p}| \cos \psi.$$

Then

$$\frac{(\mathbf{u} \times \mathbf{p}) \cdot (\mathbf{u} \times \mathbf{p})}{|p|^2} = \cos^2 2\theta \sin^2 \psi + \cos^2 2\theta \cos^2 \psi + \sin^2 2\theta \sin^2 \psi$$

$$= \cos^2 2\theta + \sin^2 2\theta \sin^2 \psi$$

$$= 1 - \sin^2 2\theta + \sin^2 2\theta \sin^2 \psi$$

$$= 1 - \sin^2 2\theta(1 - \sin^2 \psi)$$

$$= 1 - \sin^2 2\theta \cos^2 \psi$$

Page 91: Scattering by an Atom

Under the assumption of a small restoring force and no interaction between electrons, equation 3.13 should be corrected to

$$x_j = \frac{e}{m\omega_0^2} E_0 e^{i\omega_0 t - i2\pi k_0 \cdot r_j}.$$

Now define the dipole moment as

$$-ex_j = -\frac{e^2}{m\omega_0^2} E_0 e^{i\omega_0 t - i2\pi k_0 \cdot r_j}$$

$$\equiv p_j e^{i\omega_0 t}.$$

In other words p_j contains only the spatial part of the dipole. With this definition

$$p_j = -\frac{e^2}{m\omega_0^2} E_0 e^{-i2\pi k_0 \cdot r_j}.$$

Equation 3.8 previously defined p_e as

$$p_e = -E_0 \frac{e^2}{m\omega_0^2},$$

so that

$$p_j = p_e e^{-i2\pi k_0 \cdot r_j}.$$

This means, physically speaking, that the dipole moment of the jth electron in the atom is equal to the dipole moment of Thomson electron weighted by a phase factor depending on the spatial coordinates of the electron.

Equations 3.15 and 3.16

In equation 3.15, $E_{at.}$ is the amplitude of the electric field observed at the point R. However R_j appears in the exponent, because of the effective E at point R is the sum of various electronic contributions of index j (Fig. 2). The jth contribution to the amplitude has the form

$$(u_j \times p_j) \times u_j \frac{\omega_0^2}{c^2 R_j} e^{-i2\pi k_j \cdot R_j} = (u_j \times p_e) \times u_j \frac{\omega_0^2}{c^2 R} e^{-i2\pi k_0 \cdot r_j} e^{-i2\pi k \cdot R_j},$$

where we replaced k_j by k, although we did not substitute R for R_j (except in the denominator of $\omega_0^2 / c^2 R_j$). Then the exponential part looks like

$$e^{-i2\pi k_0 \cdot r_j} e^{-i2\pi k \cdot (R - r_j)} = e^{2\pi i (k - k_0) \cdot r_j} e^{-i2\pi k \cdot R},$$

and the total sum goes over to

$$\sum_j (u_j \times p_e) \times u_j e^{-i2\pi k \cdot R} \frac{\omega_0^2}{c^2 R} e^{2\pi i (k - k_0) \cdot r_j}.$$
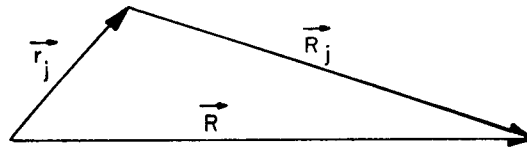
Fig. 2—Vectors from the nucleus of an atom and
its jth electron

Looking at the similarity between this and equation 3.10, we can write equation 3.16:

$$E_{at.} = E_e \sum_j e^{is \cdot r_j}, \quad s \equiv 2\pi(k - k_0).$$

This means that the amplitude $E_{at.}$ at the observation point R is the same as that of an electron in an electric field, multiplied by a phase factor $e^{is \cdot r_j}$ which is summed over all electrons in the atom.

The "interference effects" referred to at the end of page 92 may be observed not only for coherent beams from regular arrays, arising from crystal structure, but also from instantaneously incoherent beams. The only difference is that in the former these effects remain detectable through time but in the latter they disappear within a time comparable to the inverse frequency of the interacting photons. We are here concerned with only those effects that show up after time averaging, namely, structure-dependent, steady-state effects.

Page 93: Classical Assumption of Independent Probabilities

The classical assumption of independent distribution functions σ_j obviously would not hold in the quantum-mechanical treatment of the problem, because the Pauli exclusion principle would impose an additional constraint on the electronic wave functions or associated probabilities.

Page 93: Coherent Scattering

The incoherent scattering is obtained only after the *coherent* scattering and *total* scattering are written down:

$$I(\text{inc.}) = I(\text{tot.}) - I(\text{coh.}).$$

To obtain the coherent scattering, first the instantaneous *amplitudes* of equation 3.16 are averaged, whereas to obtain the *total* scattering the instantaneous *intensity* expression is averaged.

The mean amplitude in equation 3.17 is obtained by summing the amplitudes of various electrons, each one of which contributes to the sum in the form of equation 3.18. Note that averaging the quantity is the same as integrating the probability (σ_j) over the entire volume. The phase factor $e^{is \cdot r_j}$ has to be included for each term.

Equation 3.20

The second equality in equation 3.20 results from the fact that for $i = j$ the value of the double integral equals 1. There are Z terms in this integral (for the Z electrons with $i = j$. Only the terms with $i \neq j$ need by calculated. Note that since

$$\varphi_j \equiv \int \sigma_j e^{i\mathbf{s}\cdot\mathbf{r}_j} \, dv,$$

then

$$\varphi_j^* \equiv \int \sigma_j e^{-i\mathbf{s}\cdot\mathbf{r}_j} \, dv.$$

Derivation of Equation 3.21

In the derivation of equation 3.21 we must show that

$$\sum_{j \neq k}\sum \varphi_j \varphi_k^* - \left|\sum_j \varphi_j\right|^2 = -\sum_j |\varphi_j|^2.$$

We can write

$$\left|\sum_j \varphi_j\right|^2 = (\varphi_1 + \varphi_2 + \cdots \varphi_z)(\varphi_1^* + \varphi_2^* + \cdots + \varphi_z^*)$$

$$= \varphi_1\varphi_1^* + \varphi_1\varphi_2^* + \cdots + \varphi_z\varphi_z^*$$

$$= |\varphi_1|^2 + \varphi_1\varphi_2^* + \varphi_2\varphi_1^* + \cdots + |\varphi_2|^2 + \cdots + |\varphi_z|^2$$

$$= \sum_{j \neq k}\sum \varphi_j\varphi_k^* + \sum_j |\varphi_j|^2.$$

Therefore

$$\sum_{j \neq k}\sum \varphi_j\varphi_k^* - \left|\sum_j \varphi_j\right|^2 = -\sum_j |\varphi_j|^2.$$

Page 93: Sentence Following Equation 3.21

Aside from a factor of $c/8\pi$ the total intensity is the average of the squared amplitudes (mean square amplitude). The coherent scattering is the squared mean amplitude (as we noted under "Page 93: Coherent Scattering").

Page 94: Definition of Atomic Scattering Power

From equation 3.17 the definition of f^0 on page 94 gives

$$f^0 = \frac{\text{atomic amplitude}}{\text{electronic amplitude}} \quad \frac{|E_e| \sum_j \varphi_j}{|E_e|} = \sum_j \varphi_j.$$

This expression is good only for high-frequency x rays.

Equation 3.23

The element of volume in spherical symmetry is $4\pi r^2 \, dr$. When $\rho(r)$ (probability per unit volume) is given, the number of electrons between r and $r + dr$ becomes

$$\rho(r)4\pi r^2 \, dr \equiv U(r) \, dr,$$

where

$$U(r) \equiv 4\pi r^2 \rho(r)$$

and thus

$$\rho(r) = \frac{U(r)}{4\pi r^2}.$$

Page 95: The Atomic Scattering Power

Unlike section 3, in section 4 two other forces are now added to the equation of motion: the centripetal force and a velocity-dependent force. Both have minus signs, and they tend to decrease the effect of the applied force

$$-\frac{e}{m} E_0 e^{i\omega_0 t - i2\pi k_0 \cdot r_j}.$$

Again, we must solve the ordinary second-order differential equation 3.27 and obtain equation 3.28. Thus equation 3.29 is the revised expression for atomic scattering power for lower energy x rays.

Page 96

Equation 3.31 is written in a purely formal manner. It implies that the scattering power f contains an imaginary part due to the radiation damping, and a real part which may be split between f^0 (high-frequency limit) and the binding-force term $m\omega_j^2 x_j$. Equation 3.31 can also be written as

$$f = f^0 + \sum_j \varphi_j(\xi_j + i\eta_j) = \sum_j \varphi_j(1 + \xi_j + i\eta_j).$$

Section 5: First Paragraph

The vector a_i is the lattice parameter, and x_i is a number defining a fraction of this parameter. In the definition of structure factor (scattering power of a unit cell) the same provisions apply as in the atomic scattering factor.

Equation 3.32

In Equation 3.32 $\Omega(r)$ is a single function (distribution function), whose Fourier components are Ω_H. These are related to each other by the Fourier reciprocity theorem.

Equation 3.36

Equation 3.36 is analogous to equation 3.22.

Equation 3.38

Again, equation 3.38 states that the structure factor F^0 is the sum of individual scattering powers of atoms, each of which is multiplied by a phase factor. Particular note should be taken of the remarks following this equation.

Equation 3.44

For a unit cell with large or appreciable anomalous dispersion, the expression for F (not F^0 as in equation 3.38) is

$$F = \sum_k f_k e^{is \cdot r_k},$$

where f_k is the scattering power for the kth atom and is given by the expression

$$f_k = \sum_j (1 + \xi_j + i\eta_j)\varphi_j^{(k)}.$$

Equation 3.31 is the same expression without the superscript k.

Equation 3.45

When the distance R is large compared with the crystal dimensions, the waves arriving at the observation point are "plane." The "plane-wave approximation" does not, obviously, hold for very small R. In the way the phase factor $e^{i\mathbf{s}\cdot\mathbf{A}L}$ comes in the expression, the inherent assumption is that various unit cells in this crystallite radiate with the same strength aside from the geometrical phase factor. No absorption or other dynamical effects are included.

Equation 3.47

In equation 3.46 the first of the three summations on the right is

$$\sum_{L_1=0}^{N_1-1} e^{iL_1\mathbf{s}\cdot\mathbf{a}_1} = \sum_{L_1=0}^{N_1-1}\left[e^{iL_1\mathbf{s}\cdot\mathbf{a}_1}\left(\frac{e^{i\mathbf{s}\cdot\mathbf{a}_1}-1}{e^{i\mathbf{s}\cdot\mathbf{a}_1}-1}\right)\right]$$

$$= \frac{\displaystyle\sum_{L_1=0}^{N_1-1}\left[e^{i(L_1+1)\mathbf{s}\cdot\mathbf{a}_1}-e^{iL_1\mathbf{s}\cdot\mathbf{a}_1}\right]}{e^{i\mathbf{s}\cdot\mathbf{a}_1}-1}$$

$$= \frac{e^{iN_1\mathbf{s}\cdot\mathbf{a}_1}-1}{e^{i\mathbf{s}\cdot\mathbf{a}_1}-1}.$$

Thus the product of the three summations follows as given in equation 3.47, with the summation index being $i = 1, 2, 3$.

Equation 3.49

All three Laue conditions should be satisfied simultaneously.

Equation 3.52

Equation 3.52 states that when the Laue equation is satisfied the quantity F_H (structure factor for $\mathbf{s} = \mathbf{s}_H$) can be defined as

$$F_H = \sum_k{}' f_k e^{i2\pi \mathbf{B}_H \cdot \mathbf{r}_k}.$$

Note how this equation may be evaluated for various crystal structures to give usable expressions for structure factor; see, for example, Azaroff [1] and Cullity [6].

Middle of Page 101 to Middle of Page 102

For future convenience let us correct the assumed variation in the angle 2θ by writing $2\theta + 2\varepsilon$ (rather than $2\theta + \varepsilon$) so that the angle of incidence will change to $\theta + \varepsilon$. Then let us substitute 2ε for ε everywhere. Equation 3.56 becomes

$$I_H(\varepsilon) \approx I_e |F_H|^2 N^2 e^{(-\pi/\lambda^2)4\varepsilon^2 D^2 \cos^2\theta_B}$$

and equation 3.57 becomes

$$(\varepsilon)_{1/2} \approx \sqrt{\frac{\log 2}{\pi}} \frac{\lambda}{2D \cos \theta_B}.$$

There is in principle no difference between this and equation 3.57.

Page 102: Discussion of Absorption Processes

Distinction is made here between photoelectric absorption and extinction. Our explanatory note above on equation 3.45 pointed out that absorption effects are not included in that equation.

Page 102: Primary and Secondary Extinction

It is perhaps appropriate at this point to discuss the relationship between the half width of the rocking curve and the concept of extinction.

A brief explanation of primary and secondary extinction is given by Zachariasen in Chapter 4. Here, for definition alone, we choose the Darwin model of the crystal: The bulk crystal is composed of small crystallite blocks, each block oriented at a small (misorientation) angle with respect to its neighbors. Both the block size and the misorientation angles may be assumed to follow smooth, normal distribution functions. The line shape (diffraction pattern) for each block may be assumed to have the form derived in equation 3.54.

Absorption in a perfect crystallite is made up of two distinct processes. Consider what happens when the crystal is rotated with the respect to the collimated, monochromatic beam, toward the Bragg angle θ_B. At considerable angles outside θ_B, the crystal behaves like an amorphous absorber and the penetration of the beam into the crystal may be

relatively high. If the linear absorption coefficient is μ, the "absorption distance" $1/\mu$ may reach several millimeters. As the Bragg angle is approached, a greater and greater portion of the incident photons contributes to diffraction, and simultaneously the depth of penetration is rapidly decreased. This rapid reduction of the primary beam during diffraction in perfect crystals (so-called *primary extinction*) is due to multiple reflection of the beam from neighboring planes: At each double reflection the phase of the reflected beam is 180° behind that of the incident beam. Thus it may take no more than a hundred thousand atomic layers before the amplitude of the incident beam dies out. This distance of 10^4 to 10^5 atomic layers is called the "extinction depth" (see Auleytner [7]).

Consider now what happens when an aggregate of mosaic blocks (a mosaic crystal) is made to rock around the Bragg angle. The future history of a parallel pencil of x-rays arriving at the crystal surface is determined by several factors:

- Photoelectric absorption coefficient μ

- Misorientation angle between the blocks,

- Size of the crystallites,

- "Natural" half-breadth of the perfect crystallite.

If the mosaic blocks were so large compared to the $1/\mu$ distance that no significant radiation could pass through a given block after ordinary absorption, then, by using a small beam, one should see the same half breadth for the bulk crystal as for the perfect crystallite (beam 1 in Fig. 3 is a qualitative example). If the x-ray beam covered an area consisting of several blocks, the effect of the misorientation between the crystallites should also be seen in the rocking curve by a multiple peaking, the amount of which may vary depending on the geometrical divergence of the primary beam.
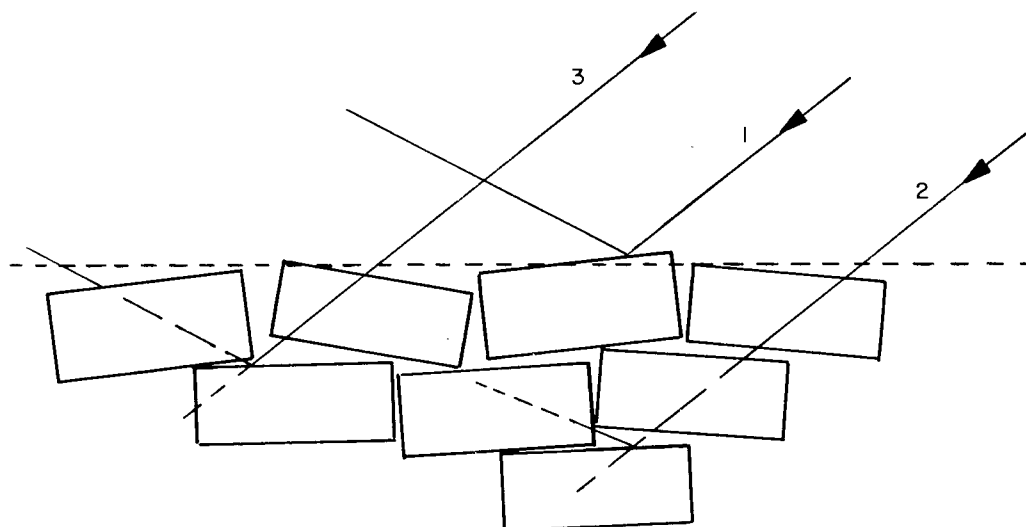
Fig. 3—Examples of beams incident from the right which are (1) totally diffracted, (2) totally absorbed, and (3) partially absorbed and partially diffracted

If the absorption distance $1/\mu$ is much larger than the average size of a given block, and if the block size in turn is larger than the extinction distance, then the beam, if not totally diffracted by a given block, may penetrate farther into the crystal, there to be diffracted by another block of proper orientation. (Beam 2 is an example in which the diffracted beam is totally absorbed.)

Finally, if the absorption distance is much larger than the extinction depth, and if this in turn is larger than the block size, part of the incident beam (beam 3) will remain unabsorbed after diffraction by each block, to arrive at lower lying crystallites.

The loss of power of primary beam *due to diffraction* by crystallites prior to the arrival of a beam at the block under consideration is called *secondary extinction.*

Equation 3.58: Absorption Coefficient μ

Note that μ here is the linear absorption coefficient. In some books(such as Jenkins and DeVries [8]) it stands for the mass absorption coefficient.

Page 103: Comments Following Equation 3.58

The reader should pay particular attention to the comments following equation 3.58 which describe the condition under which the intensity formula 3.48 holds.

Section 7

The program of section 7 is to consider the three methods of obtaining diffraction lines and to derive an expression for the intensity of a small crystal as a function of appropriate variables. Thus an initial parameter ε_1 is chosen which corresponds to the "most important" variable in each of the three methods. For example in the Laue method this corresponds to a change in the wavelength in the neighborhood of Bragg λ. If a detection surface is chosen (such as an ionization chamber), then the total power received by the detector is the integral of the intensity (function of ε_1) over the entire surface of the detector, where at the same time the variable ε_1 covers all possible ranges, hence equation 3.63. The definition of Δ at the beginning of the section (equation 3.59) is for the sake of simplicity. The integration of I_H as a function of Δ may be further simplified if an explicit form for Δ can be obtained in terms of ε_1, ε_2, and ε_3. Then the integral takes the form given in equation 3.67.

The surface element in each of the three methods can be easily evaluated. For example, in the Laue method it is obtained by "measuring" the latitude and longitude through which u_H may vary. Obviously dS is the area of a rectangle on the surface of the sphere (Fig. 3.4) whose sides are $R\,d\varepsilon_2$ and $R\,d\varepsilon_3$.

Derivation of Equation 3.65

Referring to Fig. 3.4, we fix the direction of incidence. Thus $\mathbf{u}_0 = \mathbf{u}_0^B$. Since $\Delta = \mathbf{s} - \mathbf{s}_H$, we may write

$$\mathbf{s}_H = \frac{2\pi}{\lambda_H^B} (\mathbf{u}_H^B - \mathbf{u}_0^B)$$

and

$$\mathbf{s} = \frac{2\pi}{\lambda_H} (\mathbf{u}_H - \mathbf{u}_0) = \frac{2\pi}{\lambda_H} (\mathbf{u}_H - \mathbf{u}_0^B).$$

Even though in Fig. 3.4 the directions of $\mathbf{u}_H$, $\mathbf{u}_H^B$, etc. are shown far apart, we must remember that their separation is of first order in ε_1, ε_2, ε_3, which are small quantities. From equation 3.64 we obtain

$$\frac{1}{\lambda_H} = \frac{1}{\lambda_H^B + \varepsilon_1} \approx \frac{1}{\lambda_H^B}\left(1 - \frac{\varepsilon_1}{\lambda_H^B}\right) = \frac{1}{\lambda_H^B} - \frac{\varepsilon_1}{(\lambda_H^B)^2} \; .$$

Next let us decompose the unit vectors $\mathbf{u}_H^B$, $\mathbf{u}_0^B$, $\mathbf{u}_H^0$ along the set of axes τ_1, τ_2, τ_3. The vector $\mathbf{u}_H^8$ is in the $\tau_1\tau_2$ plane. Therefore

$$\mathbf{u}_H^B = \cos 2\theta \; \boldsymbol{\tau}_1 + \sin 2\theta \; \boldsymbol{\tau}_2.$$

The vector $\mathbf{u}_0^B$ is oriented along $\boldsymbol{\tau}_1$:

$$\mathbf{u}_0^B = \boldsymbol{\tau}_1.$$

The vector $\mathbf{u}_H$ has all three components; the $\boldsymbol{\tau}_3$ component is

$$|\mathbf{u}_H| \sin \varepsilon_2 \boldsymbol{\tau}_3 = \sin \varepsilon_2 \boldsymbol{\tau}_3.$$

Its projection on the $\tau_1\tau_2$ plane is

$$|\mathbf{u}_H| \cos \varepsilon_2 = \cos \varepsilon_2.$$

Therefore we have

$$\mathbf{u}_H = \cos \varepsilon_2[\cos(2\theta + \varepsilon_3)]\boldsymbol{\tau}_1 + \cos \varepsilon_2[\sin(2\theta + \varepsilon_3)]\boldsymbol{\tau}_2 + \sin \varepsilon_2 \boldsymbol{\tau}_3.$$

We expand $\cos(2\theta + \varepsilon_3)$ and $\sin(2\theta + \varepsilon_3)$ to get

$$\cos(2\theta + \varepsilon_3) = \cos 2\theta \cos \varepsilon_3 - \sin 2\theta \sin \varepsilon_3$$

$$\approx \cos 2\theta - \varepsilon_3 \sin 2\theta$$

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and

$$\sin(2\theta + \varepsilon_3) = \sin 2\theta \cos \varepsilon_3 + \cos 2\theta \sin \varepsilon_3$$

$$\approx \sin 2\theta + \varepsilon_3 \cos 2\theta.$$

Now

$$s - s_H = 2\pi(u_H - u_0^B)\left[\frac{1}{\lambda_H^B} - \frac{1}{(\lambda_H^B)^2}\right] - \frac{2\pi}{\lambda_H^B}(u_H^B - u_0^B)$$

$$= \frac{2\pi}{\lambda_H^B}(u_0 - u_H^B) - \frac{2\pi\varepsilon_1}{(\lambda_H^B)^2}(u_0 - u_0^B), \tag{1}$$

$$u_H - u_H^B = \varepsilon_2\tau_3 + \tau_1(\cos 2\theta - \varepsilon_3 \sin 2\theta) + \tau_2(\sin 2\theta + \varepsilon_3 \cos 2\theta)$$

$$- \cos 2\theta\ \tau_1 - \sin 2\theta\ \tau_2$$

$$= \varepsilon_2\tau_3 + (\tau_2 \cos 2\theta - \tau_1 \sin 2\theta)\varepsilon_3, \tag{2}$$

$$u_H - u_0^B = \varepsilon_2\tau_3 + \tau_1(\cos 2\theta - \varepsilon_3 \sin 2\theta) + \tau_2(\sin 2\theta + \varepsilon_3 \cos 2\theta) - \tau_1. \tag{3}$$

Substituting equations 2 and 3 into equation 1, eliminating all powers of ε^2 etc., we get

$$s - s_H = \frac{2\pi}{\lambda_H^B}[\varepsilon_2\tau_2 + (\tau_2 \cos 2\theta - \tau_1 \sin 2\theta)\varepsilon_3]$$

$$- \frac{2\pi}{(\lambda_H^B)^2}\{\varepsilon_1[\tau_1(\cos 2\theta - 1) + \tau_2 \sin 2\theta]\}$$

or

$$s - s_H = \frac{2\pi\varepsilon_1}{(\lambda_H^B)^2}[\tau_1(1 - \cos 2\theta) - \tau_2 \sin 2\theta] + \frac{2\pi}{\lambda_H^B}\tau_3\varepsilon_2$$

$$+ \frac{2\pi\varepsilon_3}{\lambda_H^B}(\tau_2 \cos 2\theta - \tau_1 \sin 2\theta),$$

which agrees with equation 3.65 as given in the text, except that in the text the subscript H has been dropped for convenience, since it is understood that all the equations are written for the same set of Miller indices represented by H.

Jacobians

The concept of a Jacobian is used whenever a change of variable is necessary in a multivariable integration. In the simplest case, a change of variable from x to y, say, when $y = f(x)$, is effected in the following way:

$$dy = \frac{\partial y}{\partial x} \, dx.$$

Thus, in an integration with respect to x, the differential dx may be changed to dy if it is rewritten as

$$dx = \frac{1}{\partial y / \partial x} \, dy = \frac{\partial x}{\partial y} \, dy.$$

When the number of variables is more than one, the Jacobian may be shown to take the form of a determinant. For example, the three variables y $\{y, y_2, y_3\}$ may replace x $\{x_1, x_2, x_3\}$ by introducing the Jacobian

$$J(y, x) \equiv J\!\left(\frac{\partial y_i}{\partial x_j}\right) = \begin{vmatrix} \dfrac{\partial y_1}{\partial x_1} & \dfrac{\partial y_1}{\partial x_2} & \dfrac{\partial y_1}{\partial x_3} \\[2mm] \dfrac{\partial y_2}{\partial x_1} & \dfrac{\partial y_2}{\partial x_2} & \dfrac{\partial y_2}{\partial x_3} \\[2mm] \dfrac{\partial y_3}{\partial x_1} & \dfrac{\partial y_3}{\partial x_2} & \dfrac{\partial y_3}{\partial x_3} \end{vmatrix}.$$

Consider now a vector function $\boldsymbol{\Delta}$ decomposable along the three coordinates τ_1, τ_2, τ_3. The Jacobian which transforms the coordinates from $\varepsilon_1, \varepsilon_2, \varepsilon_3$ to p_1, p_2, p_3 (equation 3.59) can be written in a simple form, with the aid of the rules of expansion of determinants. For this purpose let us consider the derivative of the vector function $\boldsymbol{\Delta}(\varepsilon_1, \varepsilon_2, \varepsilon_3)$ or, in general, $\boldsymbol{\Delta}(x_1, x_2, x_3)$ as a three-component vector in a rectangular coordinate system:

$$\frac{\partial \boldsymbol{\Delta}}{\partial x_i} = \frac{\partial \Delta_1}{\partial x_i}\, \mathbf{e}_1 + \frac{\partial \Delta_2}{\partial x_i}\, \mathbf{e}_2 + \frac{\partial \Delta_3}{\partial x_i}\, \mathbf{e}_3$$

where $\Delta_1, \Delta_2, \Delta_3$ are the components of $\boldsymbol{\Delta}$ along the unit vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$. Without being too concerned over the mathematical rigor, we may formally regard

$$\frac{\left(\dfrac{\partial \Delta_k}{\partial x_i}\right)}{\left(\dfrac{\partial \Delta_k}{\partial y_i}\right)} \text{ as "equivalent" to } \frac{\partial y_i}{\partial x_j}\,,$$

assuming $\boldsymbol{\Delta}$ can be expressed in terms of both x and y. Because of the implicit relationship between x and y (or ε_i and p_i in our problem) we may furthermore set

$$\frac{J\!\left(\dfrac{\partial \boldsymbol{\Delta}}{\partial p_i}\right)}{J\!\left(\dfrac{\partial \boldsymbol{\Delta}}{\partial \varepsilon_i}\right)} \text{ as equivalent to } J\!\left(\frac{\partial \varepsilon_i}{\partial p_i}\right).$$

The reader may use the expansion of a three-by-three determinant and prove to himself that

$$J\left(\frac{\partial \Delta}{\partial x_i}\right) = \frac{\partial \Delta}{\partial x_1} \cdot \left(\frac{\partial \Delta}{\partial x_2} \times \frac{\partial \Delta}{\partial x_3}\right),$$

where in that determinant each row contains the components of the derivatives $\partial \Delta / \partial x_i$.

Now, to evaluate equations 3.68a and 3.68b, remember some simple rules on cross and dot products:

$$\boldsymbol{\tau}_1 \times \boldsymbol{\tau}_1 = 0, \qquad \boldsymbol{\tau}_1 \times \boldsymbol{\tau}_2 = \boldsymbol{\tau}_3, \qquad \boldsymbol{\tau}_2 \times \boldsymbol{\tau}_1 = -\boldsymbol{\tau}_3, \qquad \text{etc.}$$

$$\tilde{\boldsymbol{\tau}}_1 \cdot \boldsymbol{\tau}_1 = 1, \qquad \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 = 0, \qquad \text{etc.}$$

To evaluate the Jacobian $(\partial \Delta / \partial \varepsilon_1) \cdot [(\partial \Delta / \partial \varepsilon_2) \times (\partial \Delta / \partial \varepsilon_3)]$:

$$\frac{\partial \Delta}{\partial \varepsilon_1} = \frac{2\pi}{(\lambda_H^B)^2} [\boldsymbol{\tau}_1 (1 - \cos 2\theta_B) - \boldsymbol{\tau}_2 \sin 2\theta_B],$$

$$\left(\frac{\partial \Delta}{\partial \varepsilon_2} \times \frac{\partial \Delta}{\partial \varepsilon_3}\right) = \left[\frac{2\pi}{\lambda_H^B} \boldsymbol{\tau}_3 \times \frac{2\pi}{\lambda_H^B} (\boldsymbol{\tau}_2 \cos 2\theta_B - \boldsymbol{\tau}_1 \sin 2\theta_B)\right]$$

$$= \frac{4\pi^2}{(\lambda_H^B)^2} (-\boldsymbol{\tau}_1 \cos 2\theta_B - \boldsymbol{\tau}_2 \sin 2\theta_B),$$

and

$$\left(\frac{\partial \Delta}{\partial \varepsilon_1}\right) \cdot \left(\frac{\partial \Delta}{\partial \varepsilon_2} \times \frac{\partial \Delta}{\partial \varepsilon_3}\right) = \frac{8\pi^3}{(\lambda_H^B)^4} [(\cos 2\theta_B - 1) \cos 2\theta_B + \sin^2 2\theta_B]$$

$$= \frac{8\pi^3}{(\lambda_H^B)^4} [\cos^2 2\theta_B + \sin^2 2\theta_B - \cos 2\theta_B]$$

$$= \frac{16\pi^3}{(\lambda_H^B)^4} \sin^2 \theta_B.$$

Equation 3.71

In equation 3.71, V is the unit cell volume, δV is the unit cell volume multiplied by $N_1 N_2 N_3$, and the notation is somewhat misleading.

Equation 3.74

The surface element given by equation 3.74 is the area of the rectangle swept by the tip of $\mathbf{u}_H$, as ε_2 and ε_3 are varied (Fig. 4):

$$dS = (R \cos \varphi d\,\varepsilon_2)Rd(\varphi + \varepsilon_3)$$

or, because φ is a fixed angle,

$$dS = R \cos \varphi d\,\varepsilon_2 Rd\varepsilon_3$$

$$= R^2 \cos \varphi d\,\varepsilon_2 d\varepsilon_3.$$
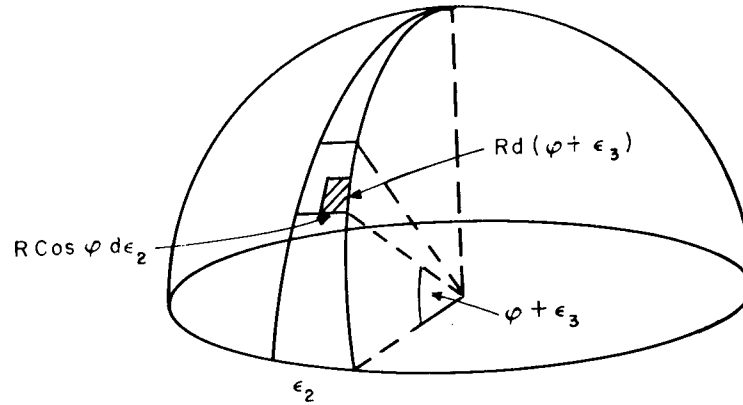
Fig. 4—Geometry pertaining to equation 3.74

Derivation of Equation 3.75

In deriving equation 3.75 we will use the expression for $s - s_H = \Delta$ as defined previously by equation 3.65. However the variable ε_1 now refers to the rotation angle from any u_0 to u_0^B. This rotation is defined in equation 3.73. Thus, with reference to Fig. 3.5,

$$u_0 = u_0^B + \varepsilon_1 \tau_3 \times u_0^B = u_0^B + \varepsilon_1 \cos \chi \tau_2$$

$$= \cos \chi \tau_1 + \varepsilon_1 \cos \chi \tau_2 - \sin \chi \tau_3,$$

$$u_0^B = \cos \chi \tau_1 - \sin \chi \tau_3,$$

$$u_H = \sin (\varphi + \varepsilon_3)\tau_3 + \cos (\varphi + \varepsilon_3)[\cos (\psi + \varepsilon_2)\tau_1 + \sin (\psi + \varepsilon_2)\tau_2],$$

$$u_H^B = \sin (\varphi) \tau_3 + \cos \varphi[\cos \psi \tau_1 + \sin \psi \tau_2],$$

$$\Delta = s - s_H = \frac{2\pi}{\lambda} [(u_H - u_0) - (u_H^B - u_0^B)] = \frac{2\lambda}{\lambda}(u_H - u_H^B + u_0^B - u_0).$$

Again we expand $\sin (\varphi + \varepsilon_2)$ etc. using the approximation of small ε_3:

$$\sin (\varphi + \varepsilon_3) = \sin \varphi + \varepsilon_3 \cos \varphi,$$

$$\cos (\varphi + \varepsilon_2) = \cos \varphi - \varepsilon_3 \sin \varphi,$$

$$\cos(\psi + \varepsilon_2) = \cos\psi - \varepsilon_2 \sin\psi,$$

$$\sin(\psi + \varepsilon_2) = \sin\psi + \varepsilon_2 \cos\psi.$$

Then

$$\mathbf{u}_H = \boldsymbol{\tau}_3(\sin\varphi + \varepsilon_3 \cos\varphi) + \boldsymbol{\tau}_1(\cos\varphi - \varepsilon_3 \sin\varphi)(\cos\psi - \varepsilon_2 \sin\psi)$$

$$+ \boldsymbol{\tau}_2(\cos\varphi - \varepsilon_3 \sin\varphi)(\sin\psi + \varepsilon_2 \cos\psi)$$

$$= \boldsymbol{\tau}_3 \sin\varphi + \boldsymbol{\tau}_3\varepsilon_3 \cos\varphi + \boldsymbol{\tau}_1(\cos\varphi \cos\psi - \varepsilon_2 \sin\psi \cos\varphi - \varepsilon_2 \sin\varphi \cos\psi)$$

$$+ \boldsymbol{\tau}_2(\cos\varphi \sin\psi - \varepsilon_2 \sin\varphi \sin\psi + \varepsilon_2 \cos\psi \cos\varphi).$$

Rearranging in terms of ε_1, ε_2, ε_3, we get

$$\boldsymbol{\Delta} = \mathbf{s} - \mathbf{s}_H = -\frac{2\pi}{\lambda} \cos\chi \boldsymbol{\tau}_2\varepsilon_1 + \frac{2\pi}{\lambda} \cos\varphi\varepsilon_2(\boldsymbol{\tau}_2 \cos\psi - \boldsymbol{\tau}_1 \sin\psi)$$

$$+ \frac{2\pi}{\lambda} \varepsilon_3(-\sin\varphi \cos\psi\boldsymbol{\tau}_1 - \sin\varphi \sin\psi\boldsymbol{\tau}_2 + \cos\varphi\boldsymbol{\tau}_3).$$

The minus sign in the ε_1 term is missing in Zachariasen's book and needs to be corrected there.

Derivation of Equation 3.77

Equation 3.77, as derived using equation 3.75, is

$$\left(\frac{\partial\boldsymbol{\Delta}}{\partial\varepsilon_1}\right) \cdot \left[\left(\frac{\partial\boldsymbol{\Delta}}{\partial\varepsilon_2}\right) \times \left(\frac{\partial\boldsymbol{\Delta}}{\partial\varepsilon_3}\right)\right] = \frac{2\pi}{\lambda} \cos\chi\boldsymbol{\tau}_2 \cdot \left[\left(-\frac{2\pi}{\lambda} \cos\varphi \sin\psi\boldsymbol{\tau}_1\right) \times \left(\frac{2\pi}{\lambda} \cos\varphi\boldsymbol{\tau}_3\right)\right]$$

$$= \left(\frac{2\pi}{\lambda}\right)^3 \cos\chi \cos^2\varphi \sin\psi.$$

In this derivation only those terms in $\boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \boldsymbol{\tau}_3$ were written out which would give non-zero contribution to the result of the cross and dot products.

Derivation of Equation 3.79

We know that $\cos 2\theta_B$ is the dot product of incident and diffracted unit vectors:

$$\mathbf{u}_0^B \cdot \mathbf{u}_H^B = \cos 2\theta_B.$$

Let us decompose $\mathbf{u}_0^B$ and $\mathbf{u}_H^B$ along the three directions $\boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \boldsymbol{\tau}_3$:

$$\mathbf{u}_0^B = (\cos \chi \boldsymbol{\tau}_1 - \sin \chi \boldsymbol{\tau}_3)$$

and

$$\mathbf{u}_H^B = (\sin \varphi \boldsymbol{\tau}_3 + \cos \varphi \cos \psi \boldsymbol{\tau}_1 + \cos \varphi \sin \psi \boldsymbol{\tau}_2).$$

Taking the dot product,

$$\mathbf{u}_0^B \cdot \mathbf{u}_H^B = (\cos \chi \boldsymbol{\tau}_1 - \sin \chi \boldsymbol{\tau}_3) \cdot (\sin \varphi \boldsymbol{\tau}_3 + \cos \varphi \cos \psi \boldsymbol{\tau}_1)$$

or

$$\cos 2\theta_B = \cos \chi \cos \varphi \cos \psi - \sin \chi \sin \varphi.$$

Two errors exist in the Zachariasen version of this result (equation 3.79).

Equation 3.80

In the powder method, the variable ε_1 is associated with the variation in the Bragg incidence angle, that is, the variation between $\mathbf{u}_0$ and $\mathbf{u}_0^B$ (Fig. 3.6). If all *directions* of incidence become equally probable, then in the calculation of intensity a required term is the probability of finding a photon at the glancing angle in the range of $\theta_B + \varepsilon_1$ and $\theta_B + \varepsilon_1 + d\varepsilon_1$ as a function of θ_B. To do this we draw the cone of axis $\mathbf{B}_H$ and semi-apex angle $(\pi/2) - (\theta_B + \varepsilon_1)$ (Fig. 5a). Now we change $\theta_B + \varepsilon_1$ to $\theta_B + \varepsilon_1 + d\varepsilon_1$ (Fig. 5b), and we calculate the fraction of photons that arrive at the apex of the cone through the small area of the circular strip. We find

$$\text{area of strip} = (2\pi a)r \, d\theta = [2\pi r \cos (\theta_B + \varepsilon_1)]r \, d\varepsilon_1$$

$$= 2\pi r^2 \cos (\theta_B + \varepsilon_1)d\varepsilon_1.$$

The total area is that of the surrounding sphere: $4\pi r^2$. The ratio of the two areas determines the probability $w \, d\varepsilon_1$ (equation 3.80):
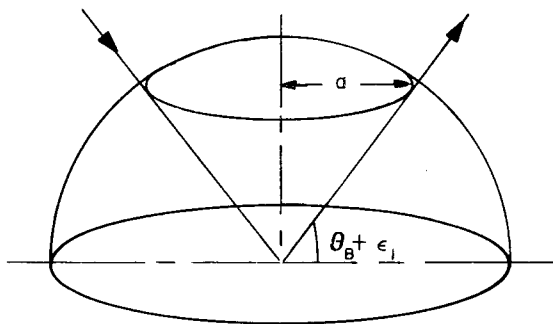
Fig. 5a—Circular cone about the vector $\mathbf{B}_H$
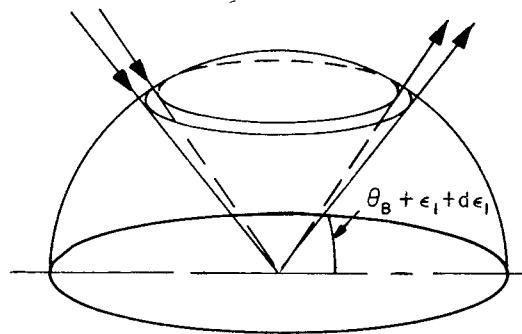
Fig. 5b—Circular cone of Fig. 5a plus an incremented cone

$$w\, d\varepsilon_1 \;=\; \frac{\text{area of strip}}{\text{area of sphere}} \;=\; \frac{2\pi r^2 \cos(\theta_B + \varepsilon_1)\, d\varepsilon_1}{4\pi r^2}$$

$$\approx \frac{1}{2}\cos\theta_B \, d\varepsilon_1 .$$

This probability factor must be multiplied into the intensity expression according to equation 3.81. The surface element for the ionization chamber is easily seen to be $R\, d\varepsilon_1\, R\, d\varepsilon_2 = R^2\, d\varepsilon_1 d\varepsilon_2$, and equation 3.81 follows.

Derivation of Equation 3.82

Calculation of Δ follows the same line as in previous sections:

$$\Delta \;=\; \frac{2\pi}{\lambda}\,[(\mathbf{u}_H - \mathbf{u}_0) - (\mathbf{u}_H^B - \mathbf{u}_0^B)] \;\equiv\; \mathbf{s} - \mathbf{s}_H ,$$

$$\mathbf{u}_H \;=\; \varepsilon_3 \boldsymbol{\tau}_3 \;+\; \cos(\theta_B + \varepsilon_2)\boldsymbol{\tau}_2 \;+\; \sin(\theta_B + \varepsilon_2)\boldsymbol{\tau}_1 ,$$

$$\mathbf{u}_H^B \;=\; \sin\theta_B \boldsymbol{\tau}_1 \;+\; \cos\theta_B \boldsymbol{\tau}_2 ,$$

$$\mathbf{u}_0 \;=\; -\sin(\theta_B + \varepsilon_1)\boldsymbol{\tau}_1 \;+\; \cos(\theta_B + \varepsilon_1)\boldsymbol{\tau}_2 ,$$

$$\mathbf{u}_0^B \;=\; -\sin\theta_B\,\boldsymbol{\tau}_1 \;+\; \cos\theta_B\,\boldsymbol{\tau}_2 ,$$

$$\cos(\theta_B + \varepsilon_2) \;\approx\; \cos\theta_B \;-\; \sin\theta_B\,\varepsilon_2 ,$$

$$\sin(\theta_B + \varepsilon_2) \;\approx\; \sin\theta_B \;+\; \varepsilon_2 \cos\theta_B ,$$

$$\Delta \;=\; \frac{2\pi}{\lambda}\,[\varepsilon_3 \boldsymbol{\tau}_3 \;+\; (\cos\theta_B - \sin\theta_B \varepsilon_2)\boldsymbol{\tau}_2 \;+\; (\sin\theta_B + \varepsilon_2 \cos\theta_B)\boldsymbol{\tau}_1]$$

$$+\; \frac{2\pi}{\lambda}\,[(\sin\theta_B + \cos\theta_B \varepsilon_1)\boldsymbol{\tau}_1 \;-\; (\cos\theta_B - \sin\theta_B \varepsilon_1)\boldsymbol{\tau}_2]$$

$$+\; \frac{2\pi}{\lambda}\,[-\cos\theta_B \boldsymbol{\tau}_2 \;-\; \sin\theta_B \boldsymbol{\tau}_1 \;-\; \sin\theta_B \boldsymbol{\tau}_1 \;+\; \cos\theta_B \boldsymbol{\tau}_2]$$

$$=\; \frac{2\pi}{\lambda}\varepsilon_1(\cos\theta_B \boldsymbol{\tau}_1 + \sin\theta_B \boldsymbol{\tau}_2) \;+\; \frac{2\pi}{\lambda}\varepsilon_2(\cos\theta_B \boldsymbol{\tau}_1 - \sin\theta_B \boldsymbol{\tau}_2) \;+\; \frac{2\pi}{\lambda}\varepsilon_3 \boldsymbol{\tau}_3 .$$

Equation 3.85

As stated by the equation directly above equation 3.85, the intensity expression is an expression of the form

$$\mathfrak{I}_H \;=\; I_0 Q \delta V ,$$

where δV is the volume of the crystal (not the unit cell volume) and Q is an expression which in the kinematical theory is well defined as soon as the experimental method is given. In the powder method, there is also the multiplicity factor which takes into account the contribution due to different atomic planes of the same type. In this connection it is important to read carefully the paragraphs of section 7. following equation 3.85.

Pages 111 and 112

Paragraphs on pages 111 and 112 contain important information regarding the differences between dynamical and kinematical theories. A large group of mathematical definitions appears here with that of the direction of $\mathbf{n}$ (page 112).

Equation 3.88

In equation 3.88 the vectors $\mathbf{D}_0$ and $\boldsymbol{\beta}_0$ inside the crystal medium replace $\mathbf{E}_0$ and $\mathbf{k}_0$ outside. Both these numbers are very nearly the same, that is, $D_0 \approx E_0^e$ and $\mathbf{k}_0 \approx \boldsymbol{\beta}_0$ subject to equation 3.89. To solve the problem two conditions must be satisfied: The first is the boundary condition that at the surface (where $\mathbf{n} \cdot \mathbf{r} = 0$)

$$\text{external incident wave} \approx \text{internal incident wave.}$$

The second condition that must hold is the "self-consistency" of internal waves (incident and diffracted).

Derivation of Equation 3.90

According to equation 3.89

$$\boldsymbol{\beta}_0 = \mathbf{k}_0(1 + \delta_0)$$

or

$$\beta_0^2 = k_0^2(1 + \delta_0)^2 \approx k_0^2(1 + 2\delta_0).$$

Now we set

$$D_0 \, e^{i\omega_0 t - i2\pi\boldsymbol{\beta}_0 \cdot \mathbf{r}} = E_0^e \, e^{i\omega_0 t - i2\pi\mathbf{k}_0 \cdot \mathbf{r}}.$$

At the boundary we have

$$e^{i\omega_0 t - i2\pi\boldsymbol{\beta} \cdot \mathbf{r}} = e^{i\omega_0 t - i2\pi\mathbf{k}_0 \cdot \mathbf{r}}$$

or

$$e^{-i2\pi\boldsymbol{\beta} \cdot \mathbf{r}} = e^{-i2\pi\mathbf{k}_0 \cdot \mathbf{r}}.$$

When two exponentials are equal, the exponents are equal, to within an additional 2π:

$$\boldsymbol{\beta}_0 \cdot \mathbf{r} = \mathbf{k}_0 \cdot \mathbf{r}.$$

Since adding a zero term on the right does not change the equality, this zero term can be in the form of a dot product with $\mathbf{r}$. Specifically,

$$\boldsymbol{\beta} \cdot \mathbf{r} = \mathbf{k} \cdot \mathbf{r} + \Delta \mathbf{n} \cdot \mathbf{r},$$

where on the surface $\mathbf{n} \cdot \mathbf{r} = 0$ and the factor Δ is necessary to make the equation valid *everywhere else:*

$$\boldsymbol{\beta}_0 = \mathbf{k}_0 + \Delta \mathbf{n}.$$

Thus outside the crystal we have $\Delta = 0$.

To obtain equation 3.90, we square the quantity $\boldsymbol{\beta}_0$ obtained above, that is, dot it into itself:

$$\beta_0^2 \approx k_0^2 + 2\Delta \mathbf{n} \cdot \mathbf{k}_0.$$

We had $\beta_0^2 = k_0^2(1 + 2\delta_0)$, so that

$$k_0^2 + 2\Delta \mathbf{n} \cdot \mathbf{k}_0 = k_0^2 + 2\delta k_0^2$$

or

$$\Delta = \frac{\delta_0 k_0^2}{\mathbf{n} \cdot \mathbf{k}_0} = \frac{\delta_0 k_0}{\mathbf{n} \cdot \mathbf{u}_0^e} = \frac{\delta_0 k_0}{\gamma_0}.$$

Therefore

$$\boldsymbol{\beta}_0 = \mathbf{k}_0^e + \Delta \mathbf{n} = \mathbf{k}_0^e + \frac{k_0 \delta_0}{\gamma_0} \mathbf{n}$$

where γ_0 is the direction cosine of the incident wave:

$$\cos \alpha = \gamma_0 = \mathbf{n} \cdot \mathbf{u}_0^e.$$

Equation 3.91

Remember that the product of the electric field and the dielectric constant defines the displacement vector.

Equation 3.92

The subscript H refers to a set of Miller indices $h_1 h_2 h_3$. One may however assign an "order" number 1, 2, 3, etc. to each set $(h_1 h_2 h_3)$ or diffracting waves in equation 3.92. Thus in equation 3.92 H may be a number like 1, 2, etc. rather than a set of three numbers. Also notice that the total diffracted wave $\mathfrak{D}$ is the sum of several $\mathbf{D}_H$ multiplied by phase factors.

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It is important to keep in mind that we are dealing with a two-wave diffraction ($\mathbf{D}_0$ and $\mathbf{D}_H$). The interested reader may search the recent literature for three-beam diffraction studies.

Equations 3.93 and 3.94

The dielectric constant of a crystal lattice is only slightly different from unity. The difference between the constant and unity is approximately $4\pi\alpha$, and this quantity is a function of the periodicity of the lattice.

The factor $4\pi\alpha$ is a scalar quantity. From optics and electricity-and-magnetism theory we know, however, that the dielectric constant has both real and imaginary parts and the imaginary part is related to the linear absorption coefficient. (We will consider more detail on this point later.) We can therefore expand the quantity $4\pi\alpha$ into a Fourier series:

$$\varepsilon \approx 1 + 4\pi\alpha = 1 + \psi,$$

where

$$\psi = \sum_H \psi_H \, e^{-i2\pi \mathbf{B}_H \cdot \mathbf{r}}.$$

Remember that $\mathbf{B}_H$ is a vector of the reciprocal lattice and the product $\mathbf{B}_H \cdot \mathbf{r}$ is dimensionless. The subscript H refers to any one of a number of possible sets of three Miller indices that give rise to diffraction. The components ψ_H of the Fourier expansion can be evaluated by the usual method based on the orthogonality of the exponential functions:

$$\psi_H = \frac{1}{V} \int \psi \, e^{i2\pi \mathbf{B}_H \cdot \mathbf{r}} \, dv$$

(the summation is over H, the integration is over dv). Thus, every vector $\mathbf{B}_H$ or $\mathbf{s}_H$ has assigned to it a subscript H for which a component ψ_H may be defined.

Equation 3.95

To get equation 3.95 from equations 3.41 and 3.42, we note that

$$F = -\frac{m\omega_0^2}{e^2} \int \alpha e^{i\mathbf{s}\cdot\mathbf{r}} \Omega_j \, dv$$

$$= -\frac{m\omega_0^2}{e^2} \frac{1}{4\pi} \int \psi e^{i2\pi \mathbf{B}_H \cdot \mathbf{r}} \, dv$$

$$= -\frac{m\omega_0^2 V}{e^2 4\pi} \psi_H$$

or

$$\psi_H = -\frac{4\pi e^2}{m\omega_0^2 V} F_H,$$

where we call the particular F, related to the subscript H, by the symbol F_H; that is F_H is the value of structure factor F for $\mathbf{s} = 2\pi \mathbf{B}_H$.

Equation 3.96

We have

$$n = \sqrt{\varepsilon} = \sqrt{1 + \psi} \approx 1 + \frac{1}{2}\psi,$$

where ψ is a small quantity ($\psi \ll 1$).

The real part of the refractive index is the factor responsible for dispersion (because n is a function of wavelength). The imaginary part of n leads to a phase shift in scattering or to true absorption.

Equations 3.97

We had, from equations 3.95 and 3.41

$$\psi = 4\pi\alpha = -\frac{4\pi e^2}{m\omega_0^2} \sum_j (1 + \xi_j + i\eta_j)\Omega_j$$

$$\equiv \psi' + i\psi'',$$

where

$$\psi' = -\frac{4\pi e^2}{m\omega_0^2} \sum_j (1 + \xi_j)\Omega_i$$

and

$$\psi'' = -\frac{4\pi e^2}{m\omega_0^2} \sum_j \eta_j \Omega_i.$$

The expression for index of refraction thus becomes

$$n = 1 + \frac{1}{2}\psi = 1 + \frac{1}{2}(\psi' + i\psi'') = 1 + \frac{1}{2}\psi' + i\frac{1}{2}\psi''.$$

The imaginary part of n is $1/2 \; \psi''$.

Equation 3.99

When both μ and ψ are expanded in a Fourier series, we have

$$\mu = \sum_H \mu_H e^{-i2\pi \mathbf{B}_H \cdot \mathbf{r}}$$

and

$$\psi = \sum_H \psi_H e^{-i2\pi \mathbf{B}_H \cdot \mathbf{r}},$$

with

$$\psi_H = \frac{1}{V}\int \psi e^{i2\pi \mathbf{B}_H \cdot \mathbf{r}} \, dv.$$

This implies

$$\psi_H' = \frac{1}{V}\int \psi' e^{i2\pi \mathbf{B}_H \cdot \mathbf{r}} \, dv$$

and

$$\psi_H'' = \frac{1}{V} \int \psi'' e^{i2\pi\mathbf{B}_H \cdot \mathbf{r}} \, dv.$$

If

$$\mu = -\frac{2\pi}{\lambda_0} \psi'',$$

then

$$\mu_H = -\frac{2\pi}{\lambda_0} \psi_H'' = \frac{2\pi}{\lambda_0} \frac{4\pi e^2}{m\omega_0^2} \frac{1}{V} \sum_j \eta_j \int \Omega_j e^{i2\pi\mathbf{B}_H \cdot \mathbf{r}} \, dv.$$

With $\omega_0 = 2\pi(c/\lambda)$

$$\mu_H = \frac{2e^2 \lambda_0}{mc^2 V} \sum_j \eta_j \int_V \Omega_j e^{i2\pi\mathbf{B}_H \cdot \mathbf{r}} \, dv.$$

Equation 3.100

To obtain the average coefficient, the set of values $(h_1 h_2 h_3)$ are set at zero; that is, the phase factor is 1.

Equation 3.101

The average real index of refraction is $1 + (\psi'/2)$, so that $\overline{\psi}' = \psi_0'$ can be obtained by the same method we used for equation 3.100:

$$\overline{\psi}' = \psi_0' = \psi_H'\big|_{H=0} = -\frac{4\pi e^2 F_0}{m\omega_0^2 V} = -\frac{4\pi e^2}{m\omega_0^2 V} \sum_j (1 + \xi_j) \quad \Omega_j \, dv$$

$$= -\frac{4\pi e^2}{m\omega_0^2 V} \sum_j (1 + \xi_j) Z_j,$$

where equation 3.42 is used in expressing F_0, and where

$$\int \Omega_j \, dv = Z_j$$

because it simply states that the density of electrons integrated over the entire volume should give the total number of electrons (of type j).

Equation 3.102

The first sentence of section 9B is important. The more familiar form of equation 3.102 is

$$\mathbf{V} \times (\mathbf{V} \times \mathbf{E}) = -\frac{1}{c^2} \frac{\partial^2 \mathbf{D}}{\partial t^2}$$

which may be rewritten as

$$(1 - \psi)\mathbf{E} = \varepsilon \mathbf{E} = \mathfrak{D} .$$

Derivation of Equation 3.103

Let us write

$$\mathfrak{D} = \sum_H \mathbf{D}_H\, e^{i\omega_0 t - i 2\pi \boldsymbol{\beta}_H \cdot \mathbf{r}} .$$

Then

$$(1 - \psi)\, \mathfrak{D} = e^{i\omega_0 t}\left(\sum_H \mathbf{D}_H\, e^{-i 2\pi \boldsymbol{\beta}_H \cdot \mathbf{r}} - \psi \sum_L \mathbf{D}_L\, e^{-i 2\pi \boldsymbol{\beta}_H \cdot \mathbf{r}} \right).$$

Here H and L are equivalent dummy indices. We expand ψ in a Fourier series,

$$\psi = \sum_K \psi_K\, e^{-i 2\pi \boldsymbol{\beta}_K \cdot \mathbf{r}} ,$$

and obtain equation 3.103:

$$(1 - \psi)\, \mathfrak{D} = e^{i\omega_0 t}\left[\sum_H \mathbf{D}_H\, e^{-i 2\pi \boldsymbol{\beta}_H \cdot \mathbf{r}} - \sum_L \sum_K \mathbf{D}_L\, \psi_K\, e^{-i 2\pi (\boldsymbol{\beta}_L + \boldsymbol{\beta}_K) \cdot \mathbf{r}} \right].$$

Derivation of Equation 3.104

Starting with equation 3.103, we have

$$(1 - \psi)\mathfrak{D} = e^{i\omega_0 t}\left[\sum_H \mathbf{D}_H e^{-i2\pi\boldsymbol{\beta}_H\cdot\mathbf{r}} - \sum_K \sum_L \mathbf{D}_L \psi_K e^{-i2\pi(\boldsymbol{\beta}_{K+L})\cdot\mathbf{r}}\right]$$

$$= e^{i\omega_0 t}\left[\sum_H \mathbf{D}_H e^{-i2\pi\boldsymbol{\beta}_H\cdot\mathbf{r}} - \sum_{H-L} \sum_L \mathbf{D}_L \psi_{H-L} e^{-i2\pi\boldsymbol{\beta}_H\cdot\mathbf{r}}\right]$$

$$= e^{i\omega_0 t}\left[\sum_H \mathbf{D}_H e^{-i2\pi\boldsymbol{\beta}_H\cdot\mathbf{r}} - \sum_H \mathbf{C}_H e^{-i2\pi\boldsymbol{\beta}_H\cdot\mathbf{r}}\right],$$

where

$$\sum_L \mathbf{D}_L \psi_{H-L} = \mathbf{C}_H.$$

Derivation of Equation 3.105a

From equation 3.104

$$\nabla \times [\nabla \times (1 - \psi)\mathfrak{D}] = -\boldsymbol{\beta}_H \times [\boldsymbol{\beta}_H \times (\mathbf{D}_H - \mathbf{C}_H)],$$

and from equation 3.92

$$-\frac{1}{c^2} \frac{\partial^2 \mathfrak{D}^2}{\partial t^2} = \sum_H \frac{\omega_0^2}{c^2} \mathfrak{D}_H e^{i\omega_0 t - i2\pi\boldsymbol{\beta}_H\cdot\mathbf{r}} = \frac{\omega_0^2}{c2} \mathfrak{D} = k_0^2 \mathfrak{D}.$$

Therefore,

$$-\boldsymbol{\beta}_H \times [\boldsymbol{\beta}_H \times (\mathbf{D}_H - \mathbf{C}_H)] = k_0^2 \mathbf{D}_H.$$

Derivation of Equation 3.105b

We have

$$-\boldsymbol{\beta}_H \times [\boldsymbol{\beta}_H \times (\mathbf{D}_H - \mathbf{C}_H)] = \boldsymbol{\beta}_H \times [(\mathbf{D}_H - \mathbf{C}_H) \times \boldsymbol{\beta}_H] = k_0^2 \mathbf{D}_H.$$

To expand this, we use the rule in vector products that

$$\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = \mathbf{B}(\mathbf{A} \cdot \mathbf{C}) - \mathbf{C}(\mathbf{A} \cdot \mathbf{B}),$$

so that

$$\boldsymbol{\beta}_H \times [(\mathbf{D}_H - \mathbf{C}_H) \times \boldsymbol{\beta}_H] = (\mathbf{D}_H - \mathbf{C}_H)\beta_H^2 - \boldsymbol{\beta}_H[\boldsymbol{\beta}_H \cdot (\mathbf{D}_H - \mathbf{C}_H)] = k_0^2 \mathbf{D}_H$$

or

$$-\mathbf{C}_H \beta_H^2 - \boldsymbol{\beta}_H[\boldsymbol{\beta}_H \cdot (\mathbf{D}_H - \mathbf{C}_H)] = (k_0^2 - \beta_H^2)\mathbf{D}_H.$$

Now

$$\boldsymbol{\beta}_H \cdot (\mathbf{D}_H - \mathbf{C}_H) = \boldsymbol{\beta}_H \cdot \mathbf{D}_H - \boldsymbol{\beta}_H \cdot \mathbf{C}_H = -\boldsymbol{\beta}_H \cdot \mathbf{C}_H$$

because

$$\boldsymbol{\beta}_H \cdot \mathbf{D}_H = 0$$

(which can be seen by dotting both sides of equation 3.105a into $\boldsymbol{\beta}_H$), and we have from equation 3.104a

$$-\boldsymbol{\beta}_H \cdot \mathbf{C}_H = -\boldsymbol{\beta}_H \cdot \left(\sum_L \psi_{H-L} \mathbf{D}_L \right),$$

which we insert along with equation 3.104a into our last equation in the preceding section to obtain

$$\sum_L [\psi_{H-L}(\boldsymbol{\beta}_H \cdot \mathbf{D}_L)\boldsymbol{\beta}_H - \psi_{H-L}\beta_H^2 \mathbf{D}_L] = (k_0^2 - \beta_H^2)\mathbf{D}_H.$$

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"Transverse" in the discussion following equation 3.105b means having components normal to the direction of propagation. Mathematically this is written as $\mathbf{D}_H \cdot \boldsymbol{\beta}_H = 0$, where $\boldsymbol{\beta}_H$ is the wave vector. The equation $\nabla \cdot \mathfrak{D} = 4\pi\rho$, where ρ is the charge dnesity, is one of Maxwell's equations. Using this, we get

$$\nabla \cdot \mathfrak{D} = \nabla \cdot \sum_H \mathbf{D}_H e^{i\omega_0 t - i2\pi\boldsymbol{\beta}_H \cdot \mathbf{r}}$$

$$= \boldsymbol{\beta}_H \cdot \sum_H{}' e^{i\omega_0 t - i 2\pi \boldsymbol{\beta}_H \cdot \mathbf{r}},$$

since applying the operator ($\nabla \cdot$) on the vector sum $\mathfrak{D}$ is equivalent to the product $\boldsymbol{\beta}_H \cdot \mathfrak{D}_H$, where $\boldsymbol{\beta}_H$ is the "derivative" of the exponent. Thus

$$\mathbf{D}_H \cdot \boldsymbol{\beta}_H = 0 \text{ implies } \nabla \cdot \vec{\mathfrak{D}} = 0.$$

This last equation is good for the oscillating part of the displacement vector, since the divergence of the static part is not zero.

Derivation of Equation 3.106

To solve the complicated set of equations 3.105, we must use some approximations. First let us assume that the Laue equations are not satisfied for any bector $\mathbf{B}_H$; that is, let us assume that the x-ray beam arrives at the crystal surface in such a way that the angle of incidence is not equal to any Bragg angle with a "detectable" diffraction amplitude. The only component of $\mathbf{D}$ is then $\mathbf{D}_0$. Others are "relatively" zero; that is, there is only an incident beam of displacement amplitude $\mathbf{D}_0$. With all $\mathbf{D}_H$ equal to zero, equation 3.105b will become

$$\psi_0(\boldsymbol{\beta}_0 \cdot \mathbf{D}_0)\boldsymbol{\beta}_0 - \psi_0 \beta_0^2 \mathbf{D}_0 = (k_0^2 - \beta_0^2)\mathbf{D}_0$$

(because H and L are both zero). However $\boldsymbol{\beta}_0 \cdot \mathbf{D}_0 = 0$, so that

$$-\psi_0 \beta_0^2 \mathbf{D}_0 = (k_0^2 - \beta_0^2)\mathbf{D}_0$$

or

$$(1 - \psi_0)\beta_0^2 = k_0^2$$

or

$$\beta_0^2 = \frac{k_0^2}{1 - \psi_0},$$

which is the first part of equation 3.106. Since ψ_0 is very small, we may expand this expression and get

$$\beta_0 \approx \frac{k_0}{\sqrt{1 - \psi_0}} \approx \frac{k_0}{1 - \frac{1}{2}\psi_0} \approx k_0\left(1 + \frac{1}{2}\psi_0\right),$$

which is the second part of equation 3.106. Remember that $1 + (1/2)\psi_0$ is the average refractive index.

Equation 3.107

To derive equation 3.107, rewrite equation 3.105b in the following way:

$$\sum_{L} [\psi_{M-L}(\boldsymbol{\beta}_M \cdot \mathbf{D}_L)\boldsymbol{\beta}_M - \psi_{M-L}\beta_M^2 \mathbf{D}_L] = (k_0^2 - \beta_0^2)\mathbf{D}_M.$$

Since the summation is over L, each M refers to a separate equation.

For $M = 0$,

$$\sum_{L} \psi_{-L}(\boldsymbol{\beta}_0 \cdot \mathbf{D}_L)\boldsymbol{\beta}_0 - \psi_{-L}\beta_0^2 \mathbf{D}_L = (k_0^2 - \beta_0^2)\mathbf{D}_0.$$

Since $\mathbf{D}_L = 0$ unless $\mathbf{D}_L = \mathbf{D}_H$ and $\mathbf{D}_L = \mathbf{D}_0$, we have

$$\psi_{-H}(\boldsymbol{\beta}_0 \cdot \mathbf{D}_H)\boldsymbol{\beta}_0 + \psi_0(\boldsymbol{\beta}_0 \cdot \mathbf{D}_0)\boldsymbol{\beta}_0 - \psi_{-H}\beta_0^2 \mathbf{D}_H - \psi_0\beta_0^2 \mathbf{D}_0 = (k_0^2 - \beta_0^2)\mathbf{D}_0.$$

We note that $\boldsymbol{\beta}_0 \cdot \mathbf{D}_0 = 0$ and set $\psi_{-H} \equiv \psi_{\overline{H}}$ to obtain

$$\psi_{\overline{H}}(\boldsymbol{\beta}_0 \cdot \mathbf{D}_H)\boldsymbol{\beta}_0 - \psi_{\overline{H}}\beta_0^2 \mathbf{D}_H - \psi_0\beta_0^2 \mathbf{D}_0 = (k_0^2 - \beta_0^2)\mathbf{D}_0,$$

which leads to the first of equations 3.107.

For $M \neq 0$, the right side of equation 3.105b contains D_M, which means $M = H$. Summing the terms for $L = H$ and $L = 0$, we get

$$\psi_0(\boldsymbol{\beta}_H \cdot \mathbf{D}_H)\boldsymbol{\beta}_H - \psi_0\beta_H^2 \mathbf{D}_H + \psi_H(\boldsymbol{\beta}_H \cdot \mathbf{D}_0)\boldsymbol{\beta}_H - \psi_H\beta_H^2 \mathbf{D}_0 = (k_0^2 - \beta_H^2)\mathbf{D}_H.$$

Again the first term in this expansion is zero ($\boldsymbol{\beta}_H \cdot \mathbf{D}_H = 0$), so that

$$\psi_H(\boldsymbol{\beta}_H \cdot \mathbf{D}_0)\boldsymbol{\beta}_H - \psi_H\beta_H^2 \mathbf{D}_0 - \psi_0\beta_H^2 \mathbf{D}_H = (k_0^2 - \beta_H^2)\mathbf{D}_H.$$

Since $\mathbf{D}_H$ is a linear combination of $\boldsymbol{\beta}_H$ and $\mathbf{D}_0$, it lies in the same plane as $\mathbf{D}_0$ and $\boldsymbol{\beta}_H$. Furthermore it was already shown that $\boldsymbol{\beta}_H \cdot \mathbf{D}_H = 0$; that is, $\boldsymbol{\beta}_H$ is normal to $\mathbf{D}_H$. Thus the three vectors $\boldsymbol{\beta}_H$, $\mathbf{D}_0$, $\mathbf{D}_H$ are all in one plane and arranged as shown in Fig. 6. The angle between $\mathbf{D}_0$ and $\boldsymbol{\beta}_H$ will be designated as χ.

Derivation of Equations 3.109

Approximating β_0^2 and β_H^2 according to equations 3.108, we get
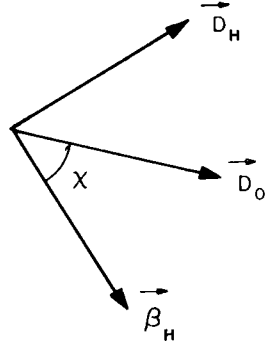
Fig. 6—Vectors of equations 3.107 (all are coplanar with the page)

$$k_0^2 - \beta_0^2(1 - \psi_0) = k_0^2 - k_0^2(1 + 2\delta_0)(1 - \psi_0)$$

$$\approx k_0^2 - k_0^2(1 + 2\delta_0 - \psi_0)$$

$$\approx -k_0^2(2\delta_0 + \psi_0)$$

and similarly

$$k_0^2 - \beta_H^2(1 - \psi_0) \approx -k_0^2(2\delta_H + \psi_0).$$

To get the first equation 3.109, we use the first equation 3.107 to write

$$\psi_{\overline{H}}(\boldsymbol{\beta}_0 \cdot \mathbf{D}_H)\boldsymbol{\beta}_0 \cdot \mathbf{D}_0 - \psi_{\overline{H}}\beta_0^2 \mathbf{D}_H \cdot \mathbf{D}_0 = -k_0^2(2\delta_0 + \psi_0)D_0^2$$

or,(remembering $\boldsymbol{\beta}_0 \cdot \mathbf{D}_0 = 0$)

$$0 - \psi_{\overline{H}}k_0^2(1 + 2\delta_0)D_H D_0 \sin \chi = -k_0^2(2\delta_0 - \psi_0)D_0^2.$$

In this equation the right side is a very small quantity, because both $2\delta_0$ and ψ_0 are small; it therefore makes sense to regard the factor $(1 + 2\delta_0)$ as almost equal to 1. Then we get

$$(2\delta_0 - \psi_0)D_0 - \psi_{\overline{H}} \sin \chi D_H = 0.$$

Similarly for the second equation 3.109, we begin with the second equation 3.107 and get

$$(2\delta_H - \psi_0)D_H - \psi_H \sin \chi D_0 = 0.$$

Equation 3.110

In equation 3.110 a distinction is made between ψ_H and $\psi_{\overline{H}}$, that is, between the two components when planes of the form $(hk\ell)$ and $(\overline{h}\overline{k}\ell)$ are considered. We will later discuss the conditions under which $\psi_{\overline{H}}$ may be set equal to ψ_H, although in most derivations we will set the two approximately equal.

Page 117:   Normal and Parallel Polarization

Let us remember the waves are transverse. Moreover, let us note that $\sin \chi$ appears in the product $\psi_{\overline{H}} \sin \chi$ only. We will set $\sin \chi = 1$ and assume normal polarization (Fig. 7). When the need arises, we will replace $\psi_{\overline{H}}$ by $\psi_{\overline{H}} \cos 2\theta$ for parallel polarization.
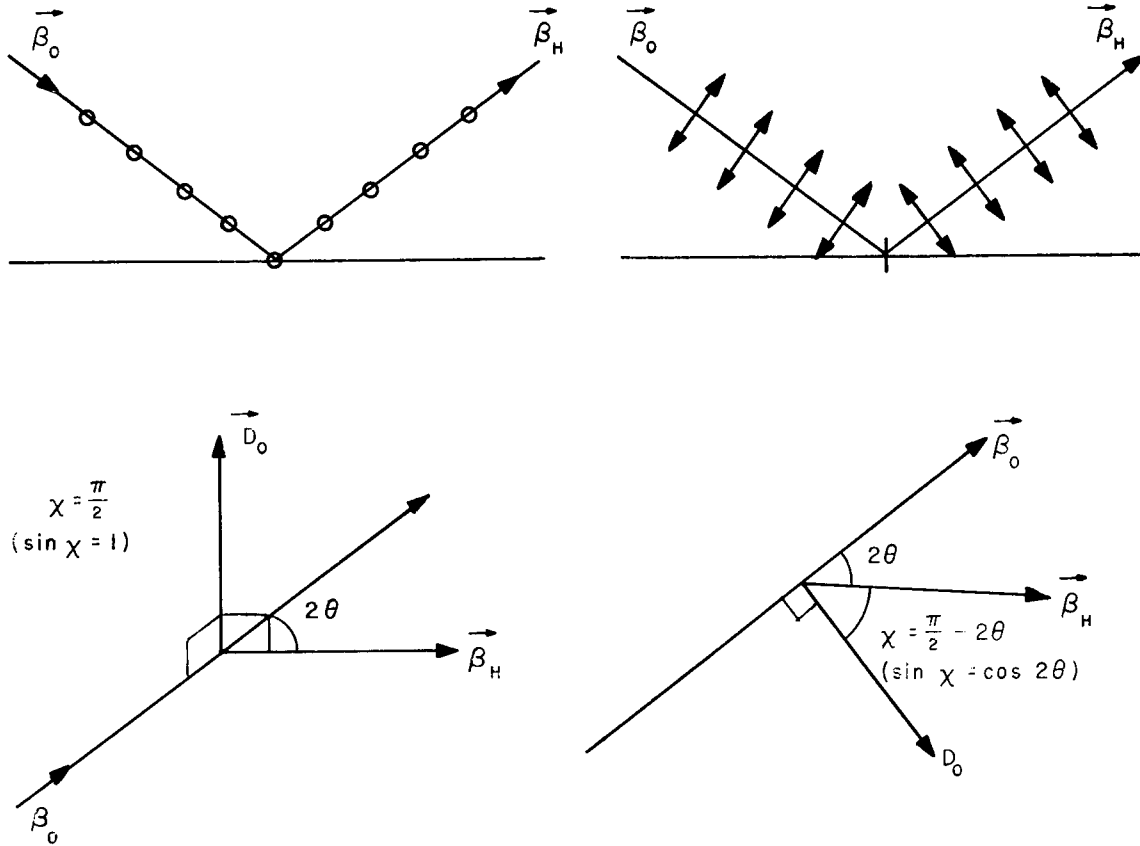
Fig. 7—Waves with parallel polarization (left half of figure) and normal polarization (right half of figure)

Derivation of Equations 3.113, 3.114a, and 3.114b

Starting with equation 3.112, we have

$$\beta_H = \mathbf{k}_0^e + \frac{k_0 \delta_0}{\gamma_0}\, \mathbf{n} + \mathbf{B}_H,$$

$$\beta_H^2 = \beta_H \cdot \beta_H = \left(\mathbf{k}_0^e + \frac{k_0 \delta_0}{\gamma_0}\, \mathbf{n} + \mathbf{B}_H \right) \cdot \left(\mathbf{k}_0^e + \frac{k_0 \delta_0}{\gamma_0}\, \mathbf{n} + \mathbf{B}_H \right)$$

$$= k_0^2 + \frac{k_0^2 \delta_0}{\gamma_0^2} + B_H^2 + 2\mathbf{u}_0 \cdot \mathbf{n}\frac{k_0^2 \delta_0}{\gamma_0} + \frac{2\delta_0 k_0 \mathbf{B}_H \cdot \mathbf{n}}{\gamma_0}$$

$$+ 2k_0^e \cdot \mathbf{B}_H.$$

Imoring $k_0^2 \delta_0^2 / \gamma_0$ in equating the preceding equation and equation 3.108, we get

$$\beta_H^2 = k_0^2(1 + 2\delta_H) = k_0^2 + B_H^2 + 2\mathbf{u}_0 \cdot \mathbf{n} \frac{k_0^2 \delta_0}{\gamma_0} + \frac{2\delta_0 k_0 \mathbf{B}_H \cdot \mathbf{n}}{\gamma_0} + 2\mathbf{k}_0^e \cdot \mathbf{B}_H$$

$$= k_0^2 + 2\delta_H k_0^2$$

or

$$\delta_H = \frac{B_H^2}{2k_0^2} + \frac{2\mathbf{k}_0 \cdot \mathbf{B}_H}{2k_0^2} + \frac{\mathbf{u}_0^e \cdot \mathbf{n}}{\gamma_0} \delta_0 + \frac{2k_0 \mathbf{B}_H \cdot \mathbf{n}}{2k_0^2 \gamma_0} \delta_0$$

or

$$\delta_H \equiv \frac{1}{2}\alpha + \frac{1}{b}\delta_0,$$

where

$$\alpha = \frac{1}{k_0^2}(B_H^2 + 2\mathbf{k}_0 \cdot \mathbf{B}_H)$$

and, since $\mathbf{u}_0^e \cdot \mathbf{n} = \gamma_0$,

$$\frac{1}{b} = 1 + \frac{\mathbf{B}_H \cdot \mathbf{n}}{\mathbf{n} \cdot \mathbf{k}_0^e}.$$

The quantities δ_0 and δ_H are related to the internal incident wave and the internal diffracted wave. The wave vectors β_0 and β_H of the internal incident and diffracted beam are related to the incident wave vector $\mathbf{k}_0$ through the pair of equations 3.108. The quantities δ_0 and δ_H are obviously small quantities, so that there is experimentally a very small difference between the various refractive indices. Equation 3.113 enables us to evaluate δ_H as a function of δ_0 and the wave vector of the incident beam. The quantity δ_0 itself is related through equations 3.108 and 3.106 to ψ_0 and thus to the average refractive index of the medium. From equations 3.113, 3.114a, and 3.114b we see that δ_H contains a part which is approximately equal to δ_0 plus another part $\alpha/2$ of the same order of magnitude.

Derivation of Equation 3.115

From equation 3.114a and the relation $\mathbf{B}_H = \mathbf{k}_H^B - \mathbf{k}_0^B$

$$b = \frac{\mathbf{n} \cdot \mathbf{k}_0^e}{\mathbf{n} \cdot (k_0^e + \mathbf{k}_H^B - \mathbf{k}_0^B)}.$$

Numerically $|k_0^e| \approx |k_0^B|$, because the wave vector does not change its value by much in diffraction. Thus

$$b = \frac{\mathbf{n} \cdot \mathbf{k}_0^B}{\mathbf{n} \cdot \mathbf{k}_H^B} = \frac{k_0^B \mathbf{n} \cdot \mathbf{u}_0^B}{k_H^B \mathbf{n} \cdot \mathbf{u}_H^B} \approx \frac{\gamma_0}{\gamma_H}.$$

Derivation of Equation 3.116

Referring to the Laue diagram in the reciprocal lattice (Fig. 3.2), we can easily write

$$\mathbf{B}_H = \mathbf{k}_H^B - \mathbf{k}_0^B.$$

Substituting this in the expression for α (equation 3.114b), we get

$$\alpha = \frac{1}{k_0^2} [(k_H^B)^2 + (k_0^B)^2 - 2\mathbf{k}_H^B \cdot \mathbf{k}_0^B + 2\mathbf{k}_0^e \cdot \mathbf{k}_H^B - 2\mathbf{k}_0^e \cdot \mathbf{k}_0^B].$$

The first two terms and the last term cancel out, as they are approximately equal and contain no cosine term. The remainder is

$$\alpha \approx \frac{1}{k_0^2} [-2k_0^2 \cos 2\theta_B + 2k_0^2 \cos(\theta + \theta_B)] \approx -2\cos 2\theta_B + 2\cos(\theta + \theta_B).$$

To get rid of $\cos 2\theta_B$, we rewrite $\theta + \theta_B$ as $2\theta_B + (\theta - \theta_B)$ or, in turn, as $2\theta_B + \Delta\theta$ and evaluate

$$\cos(2\theta_B + \Delta\theta) = \cos 2\theta_B \cos \Delta\theta - \sin 2\theta_B \sin \Delta\theta$$

$$\approx \cos 2\theta_B - (\sin 2\theta_B)(\theta - \theta_B).$$

Substituting this in the expression for α, we get

$$\alpha = 2(\sin 2\theta_B)(\theta_B - \theta).$$

Derivation of Equation 3.117

The angle between $\mathbf{u}_0$ and $\mathbf{u}_0^B$ is not $\theta_B - \theta$, as the vectors $\mathbf{u}_0$ can lie on a cone with constant θ but changing the angle between $\mathbf{u}_0$ and $\mathbf{u}_0^B$ (Fig. 8).

We must resort to some mathematical tricks for the evaluation of the quantity $(\theta_B - \theta) \sin 2\theta$ in equation 3.116. We write
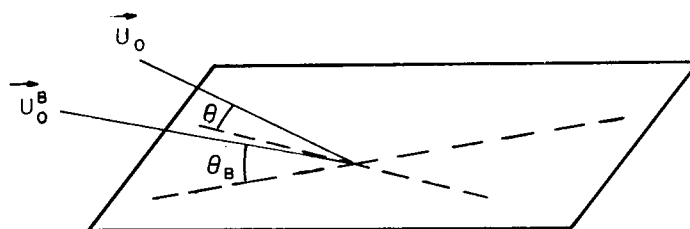
Fig. 8—Geometry pertaining to the derivation of equation 3.117

$$\theta_B + \theta = 2\theta_B - (\theta_B - \theta)$$

or

$$\cos(\theta_B + \theta) = \cos[2\theta_B - (\theta_B - \theta)].$$

Now

$$\cos(2\theta_B - (\theta_B - \theta)] = \cos 2\theta_B \cos(\theta_B - \theta) + \sin 2\theta_B \sin(\theta_B - \theta).$$

If $\theta_B \approx \theta$, then $\theta_B - \theta$ is small, so that

$$\sin(\theta_B - \theta) \approx \theta_B - \theta.$$

and

$$\cos(\theta_B - \theta) \approx 1.$$

It follows that

$$\cos(\theta_B + \theta) \approx \cos 2\theta_B + (\sin 2\theta_B)(\theta_B - \theta).$$

First, to evaluate $\cos(\theta_B + \theta)$, we consider the plane which contains the incident and diffracted beam (Fig. 9). The angle between the diffracted beam at the Bragg angle and the incident beam slightly off the Bragg angle (the angle between $\mathbf{u}_0$ and $\mathbf{u}_H^B$) is $\theta_B + \theta$. Thus, with reference to Fig. 3.5,

$$\cos(\theta_B + \theta) = \mathbf{u}_0 \cdot \mathbf{u}_H^B = \cos \chi \cos \varphi \cos \psi + \varepsilon_1 \cos \chi \cos \varphi \sin \psi - \sin \psi \sin \varphi.$$

Next $\cos 2\theta_B$ according to equation 3.79 is

$$\cos \chi \cos \varphi \cos \psi - \sin \psi \sin \varphi.$$

From these last three relations we see that

$$(\theta_B - \theta) \sin 2\theta_B = \varepsilon_1 \cos \chi \cos \varphi \sin \psi$$
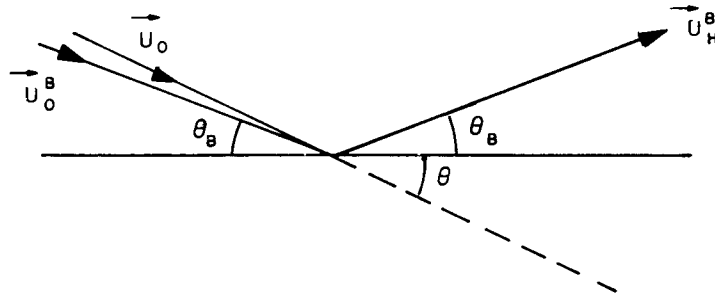
Fig. 9—Geometry of the angle between $\mathbf{u}_0$ and $\mathbf{u}_H^B$

as given in equation 3.117—resulting from the "simple consideration" mentioned in the sentence prior to the equation but rather tricky.

Derivation of Equation 3.118

Rather than expressing α in terms of θ, we consider λ as the independent variable. So (equation 3.114b),

$$\alpha = \frac{1}{k_0^2} [B_H^2 + 2\mathbf{k}_0^e \cdot \mathbf{B}_H],$$

where (from equations 3.4 and 3.2)

$$B_H^2 = \left(\frac{\mathbf{u}_H^B}{\lambda_B} - \frac{\mathbf{u}_0^B}{\lambda_B}\right) \cdot \left(\frac{\mathbf{u}_H^B}{\lambda_B} - \frac{\mathbf{u}_0^B}{\lambda_B}\right)$$

$$= \frac{1}{\lambda_B^2} + \frac{1}{\lambda_B^2} - 2\frac{1}{\lambda_B^2} \cos 2\theta_B.$$

Similarly

$$2\mathbf{k}_0^e \cdot \mathbf{B}_H = -2\frac{1}{\lambda_0}\frac{1}{\lambda_0} + 2\frac{1}{\lambda_0}\frac{1}{\lambda_B} \cos 2\theta_B.$$

Thus

$$\alpha = \lambda_0^2 \left(\frac{2}{\lambda_B^2} - \frac{2}{\lambda_B^2} \cos 2\theta_B - \frac{2}{\lambda_0 \lambda_B} + \frac{2}{\lambda_0 \lambda_B} \cos 2\theta_B\right)$$

$$= \lambda_0^2 \left[\frac{2}{\lambda_B^2} (1 - \cos 2\theta_B) - \frac{2}{\lambda_0 \lambda_B} (1 - \cos 2\theta_B)\right]$$

$$= \lambda_0^2 (1 - \cos 2\theta_B) \left[\frac{2}{\lambda_B} \left(\frac{1}{\lambda_B} - \frac{1}{\lambda_0}\right)\right]$$

$$= \frac{2\lambda_0}{\lambda_B} (1 - \cos 2\theta_0) \left(\frac{\lambda_0 - \lambda_B}{\lambda_B}\right)$$

$$\approx 4 \sin^2 \theta_B \left(\frac{\lambda_0 - \lambda_B}{\lambda_B}\right).$$

Equations 3.119 through 3.26

Equation 3.119 is derived using equation 3.113 in equation 3.110, the so-called dispersion relation, under the assumption of $\sin \chi = 1$ (normal polarization).

Substitution in equation 3.119 in terms of x (amplitude ratio, D_H/D_0) leads to equation 3.120. Either in terms of δ_0 or in terms of x the roots of the quadratic equation are given in equation 3.121 or equation 3.122. The fact that two δ's emerge from these equations implies that two internal incident waves exist. Moreover, for each x there is a ratio between $\mathbf{D}_H$ and $\mathbf{D}_0$. Hence two diffracted waves exist also. It is clear that the values of these waves should correspond to the values of δ_0' and δ_0''.

We write the total incident wave inside the medium as a two-component field (primed and double primed)

$$e^{i\omega_0 t - i2\pi \mathbf{k}_0^e \cdot \mathbf{r}}[\mathbf{D}_0' e^{-i\varphi_1 t} + \mathbf{D}_0'' e^{-i\varphi_2 t}],$$

where φ_1 and φ_2 arise from equation 3.90 in the following way.

Inside the crystal one should use $\boldsymbol{\beta}_0^e$, rather than $\mathbf{k}_0$, which from equation 3.90 is

$$\boldsymbol{\beta}_0^e = \mathbf{k}_0^e + \frac{k_0 \delta_0}{\gamma_0} \mathbf{n}.$$

The additive term in the exponential becomes the multiplier in the form $e^{-i\varphi_1 t}$, $e^{-i\varphi_2 t}$, with

$$\varphi_1 = 2\pi \frac{k_0 \delta_0'}{\gamma_0},$$

$$\varphi_2 = 2\pi \frac{k_0 \delta_0''}{\gamma_0},$$

and with

$$t = \mathbf{n} \cdot \mathbf{r}.$$

The quantity $\mathbf{n} \cdot \mathbf{r}$ defines the vertical distance from the origin to the point of observation.

It is obvious that the diffracted beam has the same form, the only difference being in the addition of $\mathbf{B}_H$ to $\mathbf{k}_0^e$ in the numerator and multiplication of x_1 and x_2 (amplitude ratios) by external amplitudes. (Remember $\mathbf{D}_H = x\mathbf{D}_0$.)

Equation 3.127

The question of the boundary condition is rather involved and is broken down into "Laue" and "Bragg" cases. However, the only additional boundary condition which can be written down is the equality of amplitudes at $\mathbf{n} \cdot \mathbf{r} = 0$ (crystal surface). Here the incident wave outside is E_0^e and that inside is the sum $D_0' + D_0''$, so that $D_0' + D_0'' = E_0^e$.

Section 10: First Paragraph

Comments on the sign of b should be read carefully.

Equation 3.129

Substituting $t = \mathbf{n} \cdot \mathbf{r} = 0$ in equation 3.125 and setting the quantity equal to 0, we get 3.128:

$$x_1 D_0' + x_2 D_0'' = 0.$$

This together with equation 3.127 gives us

$$D_0' = \frac{x_2}{x_2 - x_1} E_0^e, \qquad D_0'' = -\frac{x_1}{x_2 - x_1} E_0^e.$$

Equations 3.130 and 3.131

The notations I_e^0, I_0^e have both an advantage and a disadvantage. First, they are confusing as to which is the transmitted incident and which is the external incident wave. They are at the same time mnemonically useful: interchanging e and 0 is like interchanging the incident and transmitted waves in the Laue case.

The easiest way to remember the symbolism is to think of the ordinary I_0 as the original beam intensity and of the superscript e as denoting "external." To get equation 3.130, write

$$\frac{I_H}{I_0} = \frac{|x_1 \mathsf{D}_0' e^{-i\varphi_1 t} + x_2 \mathsf{D}_0'' e^{-i\varphi_2 t}|^2}{|E_0^e|^2}$$

and

$$(x_0' D_0' e^{-i\varphi_1 t} + x_2 D_0'' e^{-i\varphi_2 t})(x_1 D_0' e^{-i\varphi_1 t} + x_2 D_0'' e^{-i\varphi_2 t})^*$$

$$= \left| \frac{x_1 x_2}{x_2 - x_1} \right|^2 (e^{-i\varphi_1 t} - e^{-i\varphi_2 t})(e^{-i\varphi_1 t} - e^{-i\varphi_2 t})^* |E_0^e|^2$$

$$= \left| \frac{x_1 x_2 (c_1 - c_2)}{x_2 - x_1} \right|^2 |E_0^e|^2$$

where

$$c_1 = e^{-i\varphi_1 t}$$

and

$$c_2 = e^{-i\varphi_2 t}$$

In the same fashion equation 3.131 can be derived for the transmitted intensity.

Derivation of Equation 3.133

Equation 3.133 is obtained by working out equation 3.130:

$$\frac{I_H}{I_0} = \left| \frac{x_1 x_2 (c_1 - c_2)}{x_2 - x_1} \right|^2$$

In deriving equation 3.133, one must remember that the quantity I_H/I_0 is *real*. This means that the expression inside the vertical lines in equation 3.130 must *first* be expanded all the way to separate its real and imaginary parts. That expanded expression is then multiplied by its complex conjugate.

The quantities x_1 and x_2 are the two roots of the quadratic equation 3.120. From elementary relations of the quadratic equations we know that if

$$ax^2 + bx + c = 0,$$

then

$$(x_1 + x_2) = -\frac{b}{a},$$

$$x_1 x_2 = \frac{c}{a},$$

and

$$x_1 - x_2 = x_+ - x_- = \frac{\sqrt{b^2 - 4ac}}{a}.$$

Here we have

$$x_1 x_2 = -\frac{b \psi_H}{\psi_{\overline{H}}}.$$

Hence

$$|x_1 x_2|^2 = b^2 \left| \frac{\psi_H}{\psi_{\overline{H}}} \right|^2 = \frac{b^2 |\psi_H|^2}{|\psi_{\overline{H}}|^2}.$$

The quantity $x_2 - x_1$ is the difference between the two roots, and from equation 3.122 we find

$$|x_2 - x_1|^2 = \left| \frac{2\sqrt{q + z^2}}{\psi_{\overline{H}}} \right|^2 = \frac{4|q + z^2|}{|\psi_{\overline{H}}|^2}.$$

Hence

$$\left| \frac{x_1 x_2 (c_1 - c_2)}{x_2 - x_1} \right|^2 = \left| \frac{b^2 \psi_H^2 \psi_{\overline{H}}^2}{\psi_{\overline{H}}^2 \cdot 4|q + z^2|} \right| |c_1 - c_2|^2$$

$$= \frac{b^2 |\psi_H|^2}{4|q + z^2|} |c_1 - c_2|^2.$$

It remains to calculate $|c_1 - c_2|^2$. Be definition

$$c_1 \equiv e^{-i\varphi_1 t 0}, \qquad c_2 \equiv e^{-i\varphi_2 t 0},$$

where

$$\varphi_1 = 2\pi \frac{k_0 \delta_0'}{\gamma_0}, \qquad \varphi_2 \equiv 2\pi \frac{k_0 \delta_0''}{\gamma_0},$$

in which

$$\delta_0' = \frac{1}{2}(\psi_0 - z + \sqrt{q + z^2}),$$

$$\delta_0'' = \frac{1}{2}(\psi_0 - z - \sqrt{q + z^2}).$$

Before $|c_1 - c_2|^2$ can be calculated, c_1 and c_2 have to be written out explicitly in real and imaginary parts; that is, z and $\sqrt{q + z^2}$ must be separated into real and imaginary parts, where we have from equation 3.123

$$z = \frac{1 - b}{2}\psi_0 + \frac{b}{2}\alpha$$

and we define $\sqrt{q + z^2} = v + iw$ (regardless of the values of q and z). Thus

$$c_1 = e^{-(i2\pi k_0 \delta_0'/\gamma_0)t 0} = e^{-ia(\psi_0 - z + \sqrt{q + z^2})}$$

(where $a \equiv \pi k_0 t_0 / \gamma_0$) or

$$c_1 = e^{-ia[\psi_0' + i\psi_0'' - (z_{re} + iz_{im}) + v + iw]},$$

in which

$$z_{re} = \frac{1 - b}{2}\psi' + \frac{b}{2}\alpha$$

and

$$z_{\text{im}} = \frac{1-b}{2}\,\psi_0''.$$

We can write

$$\psi_0' + i\psi_0'' - (z_{\text{re}} + iz_{\text{im}}) + v + iw = \psi_0' - z_{\text{re}} + v + i\left(\psi_0'' - \frac{1-b}{2}\,\psi_0''\right) + iw$$

$$\equiv \xi + i\left(\frac{1+b}{2}\,\psi_0'' + w\right)$$

with $\xi \equiv \psi_0' - z_{\text{re}} + v$, so that

$$c_1 = e^{-ia\xi}e^{a[(1/2)(1+b)\psi_0''+w]}.$$

Here $a\xi$ and $a[(1/2)(1+b)\psi_0'' + w]$ are real quantities. Similarly

$$c_2 = e^{-ia(\psi_0'+i\psi_0''-z-v-iw)},$$

where

$$\psi_0' + i\psi_0'' - z - v - iw = \psi_0' - z_{\text{re}} - v - iz_{\text{im}} + i\psi_0'' - iw$$

$$\equiv \eta + i\left(\psi_0'' - \frac{1-b}{2}\,\psi_0'' - w\right)$$

$$= \eta + i\left(\frac{1+b}{2}\,\psi_0'' - w\right),$$

with $\eta \equiv \psi_0' - z_{\text{re}} - v$, so that

$$c_2 = e^{-ia\eta}e^{a[(1/2)(1+b)\psi_0''-w]}.$$

We evaluate

$$\frac{1+b}{2} \approx \frac{1+\dfrac{\gamma_0}{\gamma_H}}{2} = \frac{\gamma_H + \gamma_0}{2\gamma_H} \equiv \rho.$$

Now

$$|c_1 - c_2|^2 = [e^{-ia\xi}e^{a(\rho\psi_0''+w)} - e^{-ia\eta}e^{a(\rho\psi_0''-w)}][e^{ia\xi}e^{a(\rho\psi_0''+\psi)} - e^{ia\eta}e^{a(\rho\psi_0''-w)}]$$

$$= e^{2a(\rho\psi_0''+w)} + e^{2a(p\psi_0''-w)} - e^{ia(\xi-\eta)}e^{2a\rho\psi_0''} - e^{ia(\eta-\xi)}e^{2a\rho\psi_0''}$$

$$= e^{2a\rho\psi_0''}(e^{2aw} + e^{-2aw} - e^{ia2v} - e^{-ia2v})$$

$$= e^{2(\pi_0 k_0 t_0/\gamma_0)[(\gamma_H+\gamma_0)/2\gamma_H]\psi_0''}(2\cosh 2aw - 2\cos 2av).$$

We define

$$e^{2\pi k_0 \psi_0''(1/2)[(\gamma_H + \gamma_0)/\gamma_H \gamma_0)]t_0} \equiv e^{-\mu_0 t},$$

where

$$t = \frac{1}{2}\left(\frac{\gamma_H + \gamma_0}{\gamma_H \gamma_0}\right)t_0 = \frac{1}{2}\left(\frac{1}{\gamma_0} + \frac{1}{\gamma_H}\right)t_0.$$

Next we rewrite $2(\cosh 2aw - \cos 2av)$ in terms of $\sinh^2 aw$ and $\sin^2 (av)$. We recall that

$$\cos 2\theta = \frac{e^{i2\theta} + e^{-i2\theta}}{2}$$

and

$$\sin \theta = \frac{e^{i\theta} - e^{-i\theta}}{2i},$$

so that

$$\sin^2 \theta = \frac{-e^{2i\theta} - e^{-2i\theta} + 2}{4}$$

or

$$2 \sin^2 \theta = 1 - \frac{e^{2i\theta} + e^{-2i\theta}}{2} = 1 - \cos 2\theta$$

or

$$\cos 2\theta = 1 - 2 \sin^2 \theta.$$

Similarly

$$\cosh 2\theta = \frac{e^{2\theta} + e^{-2\theta}}{2}$$

and

$$\sinh = \frac{e^{\theta} - e^{-\theta}}{2},$$

so that

$$\sinh^2 \theta = \frac{e^{2\theta} + e^{-2\theta}}{2} - 1 = \cosh 2\theta - 1$$

or

$$2 \sinh^2 \theta + 1 = \cosh 2\theta.$$

(Both these relations could have been looked up in the handbook.) Thus

$$2(\cosh 2aw - \cos 2av) = 2(2 \sinh^2 aw + 1 - 1 + 2 \sin^2 av)$$

$$= 4(\sinh^2 aw + \sin^2 av).$$

Finally

$$\frac{I_H}{I_0^e} = b^2 |\psi_H|^2 e^{-\mu_0 t} \frac{\sinh^2 aw + \sin^2 av}{|q + z^2|}$$

with

$$t = \frac{1}{2}\left(\frac{1}{\gamma_0} + \frac{1}{\gamma_H}\right) t_0.$$

In the fashion in which the quantities b, q, z are defined, it seems as though $\psi_{\overline{H}}$ is absent. Closer examination of equation 3.133 shows however that $q + z^2$ contains $\psi_{\overline{H}}$, so that the expression is not asymmetric in ψ_H or $\psi_{\overline{H}}$. As it stands equation 3.133 is quite general; there are no restrictions such as centrosymmetry of crystal structure, etc. Equation 3.113 has been used, which came about from an approximation of the form 3.108 and implies that the relationship 3.133 holds when two internal waves exist and the geometry of "near-diffraction" is satisfied. (An operationally meaningful measurement of diffracted intensity requires that in the Laue case the intensity should be evaluated at $\mathbf{n} \cdot \mathbf{r} = t_0$ whereas in the Bragg case it should be evaluated at $\mathbf{n} \cdot \mathbf{r} = 0$.)

Page 121: The Bragg Case

In the Bragg case, one assumes that the diffraction takes place toward the face of the crystal closer to the incident beam. We are not concerned with the situation in which a mixture of Laue and Bragg could take place, as this implies more than one point in the reciprocal lattice satisfying the Laue equations and interferes with our original assumption of two internal waves only. (See page 116, section 9C.) Again using the always-valid relationship 3.127, we get equations 3.136, which are similar to equations 3.129.

Equation 3.137

The quantity I_H/I_0^e for the Bragg case (equation 3.137) is evaluated at $\mathbf{n} \cdot \mathbf{r} = 0$, whereas I_0^e/I_0^e is evaluated at $\mathbf{n} \cdot \mathbf{r} = t_0$. Equation 3.137 can be derived with a little more tedium than was equation 3.133 (but along the same line), because it contains more terms. This derivation is left out of our notes.

Although this equation does not contain an explicit absorption factor $(e^{-\mu_0 t})$, this does not mean that absorption is not present, because absorption is related to the polarizability per unit volume, whose value imposes a numerical condition on ψ_H and $\psi_{\overline{H}}$. In particular, as stated at the end of the second note that follows, zero absorption means $\psi_H \psi_{\overline{H}} = |\psi_H|^2$.

Page 122: Last Paragraph

Figure 10 may clarify the geometry of incident and diffracted beams in the evaluation of the integrated power ratio. It is clear that the assumption

$$\frac{S_H}{S_0} = \frac{1}{|b|}$$

holds only for small depths of penetration. An expression could be worked out for the ratio S_H/S_0 as a function of depth of penetration. This, however, would be irrelevant to the present problem, because in most cases the beam size is indeed large enough compared to the penetration depth to satisfy the above relationship, and if the penetration depth were large, the relations $P_H = I_H S_H$ and $P_0 = I_0 S_0$ would not hold true, as the intensity would not be uniform across the beam (due to absorption), and both relations should then be replaced by some sort of volume integrals rather than simple linear products. Note also that the only case in which the cross-section areas of the incident and diffracted beam are equal occurs when the diffracting planes are parallel to the surface of the crystal.

(a)   (b)
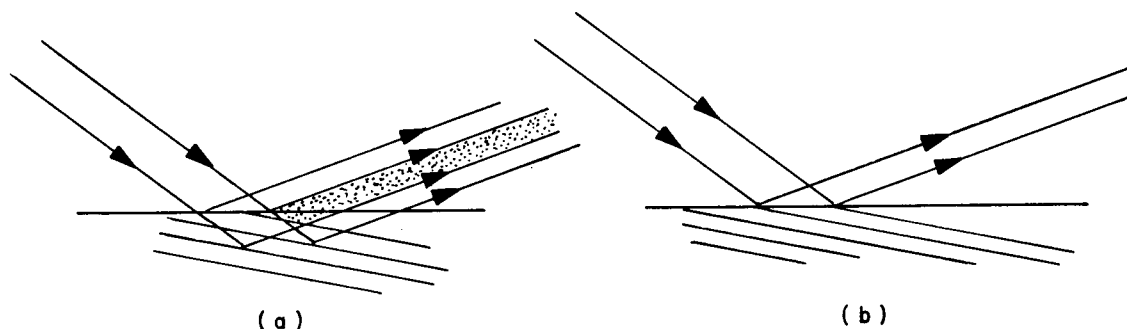
Fig. 10—Geometry of incident and diffracted beams in the evaluation of the integrated power ratio for the Bragg case: (a) Large depth of penetration and (b) Small depth of penetration

Page 123: First Paragraph of Section 11

Remember that μ_0 was obtained from equation 3.100 and depends on the imaginary part of the polarizability per unit volume. Therefore

$$\psi'' = 0, \qquad \alpha = 1 + \psi'.$$

Furthermore the Fourier coefficients are not necessarily real, but they must satisfy the condition that inverting the indices H does not change the value of ψ_H (see equation 3.94):

$$e^{i2\pi \mathbf{B}_H \cdot \mathbf{r}} \Rightarrow e^{-i2\pi \mathbf{B}_{\overline{H}} \cdot \mathbf{r}} = e^{i2\pi \mathbf{B}_H \cdot \mathbf{r}}$$

or

$$\psi_{\overline{H}} = \psi_H^*.$$

Therefore

$$\psi_H \psi_H^* = \psi_H \psi_{\overline{H}} = |\psi_H|^2.$$

Page 123: Power Ratio in the Laue Case; Derivation of Equation 3.142

With zero absorption equation 3.133 becomes

$$\frac{I_H}{I_0^e} = \frac{\sin^2 (av)}{|q + z^2|} b^2 |\psi_H|^2.$$

We convert $|\psi_H|$ to $K|\psi_H|$, where K is the polarization factor (1 or $\cos 2\theta$). With $q = b|\psi_H|^2 K^2$ and $v = \sqrt{q + z^2}$ we have

$$\frac{I_H}{I_0^e} = \frac{b^2 |\psi_H|^2 K^2 \sin^2 \left(a\sqrt{b}|\psi_H|K \sqrt{1 + \dfrac{z^2}{b|\psi_H|^2 K^2}} \right)}{K^2 b |\psi_H|^2 \left(1 + \dfrac{z^2}{b|\psi_H|^2 K^2} \right)},$$

which from the relation $P_H/P_0 = (1/|b|)(I_H/I_0)$ becomes equation 3.142, in which (definitions 3.140 and 3.141)

$$A = a\sqrt{b}|\psi_H|K, \qquad y = \frac{z}{\sqrt{b|\psi_H|^2 K^2}} = \frac{\frac{1}{2}[(1-b)\psi_0 + b\alpha]}{\sqrt{|b|}\,|\psi_H|K}.$$

From the form of equation 3.142 the variable y is dimensionless. It is related to α through the definition 3.141. However do not confuse this α with the α (polarizability) as defined in equation 3.93! The dimensionless variable y has a particular advantage over the other variables (θ, λ, ε_1) in that it makes the calculations "coordinate independent." Once the results are obtained for y, they can be easily rewritten for other variables.

Page 124

In the Bragg case it is necessary to check whether $\sqrt{q + z^2}$ is positive or negative, because $b < 0$. The separate solutions are derived in equations 3.143 and 3.144. Note the remark directly under equation 3.144.

A particular elegance of the use of the y scale is that it makes the diffraction patterns symmetrical (since changing y to $-y$ does not change the form of equations 3.142 through

3.144. On the other hand the *center* of the diffraction pattern, $y = 0$, does not necessarily corresond to θ_B but to θ_0 or λ_0 as defined below. With reference to equation 3.123

$$\frac{1-b}{2}\,\psi_0 + \frac{b}{2}\alpha = 0$$

or

$$(1-b)\psi_0 = -b\alpha.$$

From equation 3.116 we have

$$(1-b)\psi_0 = -b\alpha = 2b(\theta_0 - \theta_B)\sin 2\theta_B.$$

Therefore

$$\theta_0 = \theta_B + \frac{(1-b)\psi_0}{2b\sin 2\theta_B}.$$

Similarly from equation 3.118 we have

$$(1-b)\psi_0 = -4b\frac{\lambda_0 - \lambda_B}{\lambda_B}\sin^2\theta_B$$

or

$$\lambda_0 = \lambda_B - \frac{\lambda_B(1-b)}{4b\sin^2\theta_B}\,\psi_0.$$

Obviously $\theta_0 = \theta_B$ and $\lambda_0 = \lambda_B$ only when $b = +1$. The center of diffraction pattern corresponds to the Bragg angle only in the symmetrical Laue case. *This is not true for any other geometry.*

Page 124: Last Two Sentences

See equations 3.95, 3.100, and 3.101. Remember that ψ_0'' is zero (no absorption), so that ψ_0 is completely real.

$$\psi_0 = \psi_0' + i\psi_0''$$

Derivation of Equation 3.146a

From equation 3.131

$$\frac{I_e}{I_0} = \left|\frac{x_2 c_1 - x_1 c_2}{x_2 - x_1}\right|^2 = \frac{x_2 c_1 - x_1 c_2}{x_2 - x_1}\left(\frac{x_2 c_1 - x_1 c_2}{x_2 - x_1}\right)^*.$$

Previously we had

$$\frac{I_H}{I_0^e} = b^2 |\psi_{\overline{H}}|^2 \frac{\sin^2 av}{|q + z^2|} \,.$$

Here the denominator is obtained the same way as before

$$|x_2 - x_1|^2 = \frac{4|q + z^2|}{|\psi_{\overline{H}}|^2} \,.$$

The numerator is

$$|x_2 c_1 - x_1 c_2|^2 = x_1^2 + x_2^2 - x_1 x_2 (c_1 c_2^* + c_2^* c_1)$$

$$= x_1^2 + x_2^2 - x_1 x_2 [e^{i(\varphi_2 - \varphi_1)} + e^{i(\varphi_1 - \varphi_2)}].$$

This factorization is possible because $x = x^*$ with no absorption. Note that the φ's are real; if they were imaginary or complex the above step would have to be done more carefully! Thus

$$|x_2 c_1 - x_1 c_2|^2 = x_1^2 + x_2^2 - 2x_1 x_2 \cos [(\varphi_2 - \varphi_1) t_0],$$

where

$$(\varphi_2 - \varphi_1) t_0 = \frac{2\pi k_0 t_0}{\gamma_0} (\delta_0'' - \delta_0') = 2a(\delta_0'' - \delta_0'),$$

in which a was defined in equation 3.134. With

$$\delta_0'' - \delta_0' = \sqrt{q + z^2} \equiv v$$

we get for the numerator

$$\text{numerator} = x_1^2 + x_2^2 + 2x_1 x_2 - 2x_1 x_2 - 2x_1 x_2 \cos 2av$$

$$= |x_1 - x_2|^2 + 2x_1 x_2 (1 - \cos 2av)$$

$$= |x_1 + x_2|^2 - 4b \frac{|\psi_H|}{|\psi_{\overline{H}}|} \sin^2 av.$$

Observing the expressions above for I_H/I_0^e and I_e^0/I_0^e, we have

$$\frac{I_e^0}{I_0^e} = 1 - \frac{1}{b} \frac{I_H}{I_0^e}$$

or

$$P_e^0 = P_0^e - P_H$$

or

$$P_0^e = P_e^0 + P_H.$$

Page 125: Bottom Paragraph

See equations 3.116 and 3.118.

Equations 3.147 through 3.149

In the four relations 3.147 the ratio P_H/P_0 should first be expressed in terms of the variable with respect to which the integral is calculated. For the variable y this quantity is already worked out as equations 3.142 through 3.144. It is therefore necessary to transform the integrals for the other three variables. To avoid the difficulty of the precise definition of domain of integration, we conveniently extend the limits to $(-\infty, +\infty)$. Then the integration can be performed by multiplying each integrand by the partial derivative of the variable considered with respect to y: For example, $d\theta = (\partial\theta/\partial y)dy$, etc., where $\partial\theta/\partial y$ is then a constant and comes out of the integral sign (the relationship between all these variables is *linear*). In this fashion equation 3.148 leads to 3.149. Once again we see that only R_H^y is essential for any calculation.

Page 126: Diffraction in Thick Crystals

The power ratio 3.142 in the Laue case shows an oscillating nature that becomes more and more pronounced with increasing A. An uncertainty in the thickness equal to 10^{-3} cm or in A equal to $\pi/2$ justifies the substitution of the $\sin^2$ term by its average value $1/2$. We arrive at this uncertainty through the following estimate. We have from equation 3.140

$$A = \pi k_0 K |\psi_H| \frac{t_0}{\sqrt{\gamma_0 \gamma_H}}$$

or

$$\Delta A = \pi k_0 K |\psi_H| \frac{\Delta t_0}{\sqrt{\gamma_0 \gamma_H}}.$$

For $\Delta A = \pi/2$

$$\frac{\pi}{2} \approx \pi k_0 |\psi_H| \frac{\Delta t_0}{1}.$$

Since

$$\psi_H = \frac{4\pi e^2 F_H}{m \omega_0^2 V},$$

with

$$e = 4.8 \times 10^{-10} \text{ esu},$$

$$k_0 = 10^{19},$$

$$F_H = 10 \text{ or } 20,$$

$$V \approx (3 \text{ Å})^3 \approx 30 \times 10^{-24} \text{ cm}^3,$$

$$m = 9.1 \times 10^{-27} \text{ g},$$

this gives

$$\Delta t_0 \approx 10^{-3} \text{ cm}.$$

Equation 3.151

The half-width value is determined easily on θ and λ scales by the same method as equation 3.149.

Equations 3.152

The evaluation of $R_H^y = \pi/2$ and other R values as in equations 3.152 are the easiest for the Laue case with no absorption. These again are straightforward and will not be explained here.

Equation 3.153

The average polarization factor is the value customarily used in a simple diffraction experiment. However it should not be assumed that this value holds for various geometrical arrangements, as encountered for example in the double-crystal spectrometer.

Equation 3.154

In Equation 3.144, $\sqrt{1 - y^2}$ is physically meaningful when $|y| < 1$. Hence, as A increases, the ratio P_H/P_0 approaches unity, because both the numerator and the denominator contain $\sinh^2 A\sqrt{1 - y^2}$. For very thick crystals it follows

$$\frac{P_H}{P_0} = 1 \text{ when } |y| < 1 \quad \text{and} \quad A \gg 1.$$

We had previously (last paragraph on page 122)

$$\frac{P_H}{P_0} = \frac{1}{|b|} \frac{I_H}{I_0^e}$$

or

$$\frac{I_H}{I_0^e} = |b| = \left|\frac{\gamma_0}{\gamma_H}\right| = -\frac{\gamma_0}{\gamma_H} \quad \text{with} \quad b < 0$$

or

$$I_H\gamma_H + \gamma_0 I_0^e = 0,$$

which shows that the (algebraic) sum of inward and outward flux equals zero (total reflection). This holds for the range $|y| < 1$.

Derivation of Equation 3.155

Equation 3.155 is the result of evaluating the average P_H/P_0 for thick crystals when $|y| > 1$. We begin with the expression for P_H/P_0 given by equation 3.143:

$$\frac{P_H}{P_0} = \frac{\sin^2 A\sqrt{y^2 - 1}}{y^2 - 1 + \sin^2 A\sqrt{y^2 - 1}}.$$

This can be rewritten

$$\frac{\sin^2 A\sqrt{y^2 - 1}}{y^2 - 1 + \sin^2 A\sqrt{y^2 - 1}} = \frac{y^2 - 1 + (\sin^2 A\sqrt{y^2 - 1}) - (y^2 - 1)}{y^2 - 1 + \sin^2 A\sqrt{y^2 - 1}}$$

$$= 1 - \frac{y^2 - 1}{y^2 - 1 + \sin^2 A\sqrt{y^2 - 1}}.$$

For large A therefore we need to average the second part only. We are interested in an integral of the form

$$\frac{1}{\delta A} \int_{A_1}^{A_1 + \delta A} \frac{y^2 - 1}{y^2 - 1 + \sin^2 A\sqrt{y^2 - 1}} \, dA,$$

where δA is chosen such that the integral goes between maximum and minimum. Without setting the limits of integration and specifying the value of δA more exactly, we evaluate the indefinite integral. We let

$$y^2 - 1 = x^2, \qquad x > 0.$$

Thus

$$\frac{1}{\delta A} \int \frac{(y^2-1)dA}{y^2-1+\sin^2 A \sqrt{y^2-1}} = \frac{y^2-1}{\delta A} \int \frac{dA}{x^2+\sin^2 Ax}$$

$$= \frac{1}{x}\frac{y^2-1}{\delta A} \int \frac{d(Ax)}{x^2+\sin^2 Ax}$$

$$= \frac{y^2-1}{x\delta A} \int \frac{dz}{x^2+\sin^2 z} \; .$$

From a table of integrals

$$\int \frac{dx}{a+b\sin^2 x} = \frac{\text{sign } a}{\sqrt{(a+b)a}} \arctan\left(\sqrt{\frac{a+b}{a}}\tan bx\right)$$

or

$$\int \frac{dz}{x^2+\sin^2 z} = \frac{1}{\sqrt{x^2+1)x^2}} \arctan\left(\sqrt{\frac{x^2+1}{x^2}}\tan z\right)$$

The limits of integration were set at A_1 and $A_1 + \delta A$. After multiplication by x and re-defining the variable, the limits are $A_1 x$ and $(A_1 + \delta A)x$. Hence

$$\int \frac{dz}{x^2+\sin^2 z} = \frac{1}{\sqrt{(x^2+1)x^2}}\left\{\arctan\left[\sqrt{\frac{x^2+1}{x^2}}\tan(A_1+\delta A_1)\right]x\right.$$

$$\left. - \arctan\left(\sqrt{\frac{x^2+1}{x^2}}\tan A_1 x\right)\right]\right\} .$$

Since the value of A_1 is uncertain by an appreciable amount ($\approx \pi/2$), we choose $A_1 x$ in such a way that $\tan A_1 x = 0$. The value of the second of the two terms in the braces is then 0. For the first term in the braces we should evaluate $\tan (A_1 + \delta A_1)x$. Since $\tan A_1 x = 0$, $\tan (A_1 + \delta A_1)x = \tan (\delta A_1 x)$. The value of this quantity depends (for *each* x in the problem) on the value δA_1. We choose the smallest value in terms of x that makes the quantity $\tan (\delta A_1 x)$ a maximum (we do not care for other values of δA_1). So we must have $\delta A_1 x = \pi/2$ or $\delta A_1 = \pi/2x$. This is the value of δA_1 that gives the average of the integral, which should be evaluated between the limits A_1 and $A_1 + \delta A_1$. Reinserting the multiplier $(y^2-1)/x\delta A$ that was in front of the integral, we get

$$\frac{y^2-1}{x}\frac{\pi/2}{\pi/2x}\frac{1}{\sqrt{x^2(x^2+1)}} = \frac{y^2-1}{\sqrt{(x^2+1)x^2}} = \frac{y^2-1}{\sqrt{(y^2-1)y^2}} = \frac{\sqrt{y^2-1)}}{\sqrt{y^2}} = 1-\frac{1}{y^2} \; .$$

The complete expression for equation 3.155 is now

$$\frac{1}{\delta A_1} \int_{A_1}^{A_1+\delta A_1} \frac{P_H}{P_0} \, dA = 1 - \sqrt{1-y^2} \,.$$

The relationship $\delta A_1 = \pi/2x$ implies that for small x, that is, $y \approx 1$, δA_1 can be many times $\pi/2$. However as x, and therefore y, increases, up to $x = 1$, the value of δA_1 approaches $\pi/2$. For very large x or y, sensitivity in δA decreases to a fraction of π. It is therefore important to indicate the range of applicability of these results. Conclusions drawn from equation 3.148 are left up to the reader.

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To evaluate R_H^y, we integrate

$$\int_{-\infty}^{\infty} \frac{P_H}{P_0} dy = \int_{-\infty}^{\infty} \frac{P_H}{P_0} \, dy + \int_{-1}^{1} \frac{P_H}{P_0} \, dy + \int_{+1}^{\infty} \frac{P_H}{P_0} \, dy$$

$$= \frac{\pi}{2} - 1 + 2 + \frac{\pi}{2} - 1 = \pi.$$

Other expressions in equations 3.156 follow the same way as for equations 3.152. Note that

$$R_H^y \text{ (Bragg)} = 2R_H^y \text{ (Laue)}.$$

The reader may be able to give a simple plausibility argument for this.

Page 129, Thin Crystals

For the very thin crystal, with A very small, one of two things may occur. In the equation

$$\frac{P_H}{P_0} = \frac{\sin^2 A\sqrt{y^2+1}}{\sqrt{y^2+1}}$$

either y is small, in which case the numerator is much smaller than the unity and the ratio P_H/P_0 is negligible, or y is large, in which case $y^2 + 1 \approx y^2$ and equation 3.157 follows. The same reasoning applies to equations 3.143 and 3.144.

Comments Following Equation 3.159

The comments following equation 3.159 should be read in the light of our redefinition of half-width according our note pertaining to the middle of page 101. When D is small (so that the entire crystal plate contributes to diffraction), we may see that the definition $D = t_0 (\sin \theta_B)/|\gamma_H|$ is physically reasonable (Fig. 11).
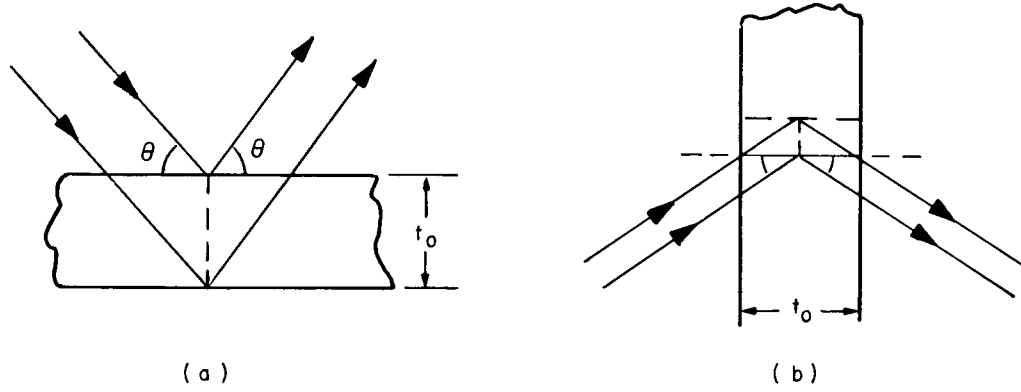
Fig. 11—Diffraction geometries for thin crystals: (a) Bragg case: $D = t_0$ and (b) Laue case:
$$D = t_0 \tan \theta_B$$

Equation 3.160

It may be seen that the total reflecting power for a "thin" crystal is a linear function of A, whereas for the thick-crystal there is no A dependence.

Equation 3.161

We write

$$A = \frac{\pi k_0 t_0}{\gamma_0} \sqrt{|b|} \, |\psi_H| = a\sqrt{|b|} \, K|\psi_H|,$$

$$K = 1 \text{ or } \cos 2\theta,$$

$$\psi_H = -\frac{4\pi e^2 F_H}{m\omega_0^2 V},$$

and

$$\psi_H = -\frac{4\pi e^2 F_H \lambda^2}{m(2\pi c)^2 V} \Rightarrow |\psi_H|^2 = \frac{1}{\pi^2} \frac{e^2}{(mc^2)^2 V^2} |F_H|^2.$$

Therefore, from the last of equations 3.160,

$$R_H^\lambda = \frac{\pi A |\psi_H| K \lambda}{\sqrt{|b|} \, 2 \sin^2 \theta_B} = \frac{\pi^2 k_0 t_0 \sqrt{|b|} \, K^2 |\psi_H|^2 \lambda}{\sqrt{|b|} \, 2(\sin^2 \theta_B)\gamma_0},$$

which becomes after taking the mean for normal and parallel polarization

$$R_H^\lambda = \frac{\pi^2 t_0}{\gamma_0} \left(\frac{1 + \cos^2 2\theta_B}{2} \right) \frac{|F_H|^2 \lambda^4}{2(\sin^2 \theta_B)\lambda^2} \left(\frac{e^2}{mc^2 V} \right)^2$$

$$= a\frac{t_0}{\gamma_0} \ .$$

In taking the mean we have written

$$\frac{1}{2}(K_\parallel^2 + K_\perp^2) \ = \ \frac{1}{2}(1 + \cos^2 2\theta_B).$$

Page 131: Top of Page

The paragraph portion at the top of page 131 contains some very important remarks regarding kinematical and dynamical theories.

Page 131: Crystals of Intermediate Thickness

Setting $y = 0$ in the Laue expression $(\sin^2 A \sqrt{1 + y^2})/(1 + y^2)$ (for the center of the diffraction pattern), we see that the value of $\sin^2 A$ increases to 1 as $A \to \pi/2$. Thereafter, it oscillates between 0 and 1. Away from the center, that is, for $y \neq 0$, the Laue expression is an oscillating function of A. for every y in the problem, the higher values of A lead to faster and faster oscillations; that is, the interference fringes squeeze together with increasing A.

Equation 3.162 Through 3.166

It is easier to develop a manageable expression for the *total* integrated intensity than for the power ratio. A familiar mathematical tool is used here: To evaluate a function $f(x)$ it may be convenient to first differentiate the function, expand the derivative in a Taylor or some other infinite series, and then reintegrate. A variation of this trick is used in deriving equation 3.165: Since we observe from equation 3.163 the similarity with the Bessel integral, differentiate equation 3.163, express the result in the Bessel function $J_0(\rho)$, and again integrate.

Equation 3.166 verifies the previous results that for the Laue (as well as the Bragg) case, small A implies $R_H^y = \pi A$, and *for the Laue case alone*, with very large A, $R_H^y = \pi/2$.

Page 133: Bragg Case

For the range $y < 1$ see equation 3.154. Again, working out the integral 3.167 for R_H^y, we find the numerical estimates for large and small A in agreement with previously derived equations.

Equation 3.169

The definition 3.169 is the same as the definition 3.140. A "strong" reflection means relatively large F_H or ψ_H. Substituting appropriate numbers for F_H (calcite etc.), we get $A = 1.7 \times 10^3 \, Kt_0/\sqrt{\gamma_0\gamma_H}$, whereas for smaller F_H we would find smaller A. The assumption that

$$A = 1.7 \times 10^3 \frac{Kt_0}{\sqrt{\gamma_0\gamma_H}} < 0.4$$

implies

$$\frac{Kt_0}{\sqrt{\gamma_0\gamma_H}} < 0.4 \frac{1}{1.7 \times 10^3} \approx 0.2 \times 10^{-3} = 2 \times 10^{-4}.$$

Thus the "effective linear dimension" increases with decreasing A. The relationship 3.169 controls the range of applicability of the thin crystal formula for strong and weak reflections.

Equations 3.170

By $\psi'_{\overline{H}}$ we mean ψ'_H with "minus H," that is, with reversed Miller indices.

Equation 3.172

See equation 3.98.

Equation 3.147

In equation 3.174 the factor $\psi_0/2$ is the same as δ_0 as shown by equations 3.90, 3.106, and 3.108. Also note the misprint: the bracket in the exponent should be dotted into **r**.

Equations 3.177

Both Fourier components of ψ' and ψ'' are in general complex. We had previously set the quantities $|\psi_H|^2$, $|\psi_{\overline{H}}|^2$, and $|\psi_H\psi_{\overline{H}}|$ equal to each other. Here however we must resolve them into real and imaginary parts. For example

$$\psi_H = |\psi'_H + i\psi''_H|^2 = (\psi'_H + i\psi''_H)(\psi'^*_H - i\psi''^*_H)$$

$$= |\psi'_H|^2 + |\psi''_H|^2 - i\psi'_H\psi''^*_H + i\psi''_H\psi'^*_H.$$

Now

$$i\psi'_H \psi''^*_H + (i\psi'_H \psi''^*_H)^* = 2\,\text{Re}\,(i\psi'_H \psi''^*_H).$$

We have

$$\psi'^*_H = (\psi'_{H_r} + i\psi'_{H_i})^* = \psi'_{H_r} - i\psi'_{H_i}; \qquad \psi''_H = \psi''_{H_r} + i\psi''_{H_i}$$

and

$$\text{Re}\,(i\psi'_H \psi''^*_H) = \text{Re}\,[i(\psi'_{H_r} - i\psi'_{H_i})(\psi''_{H_r} + i\psi''_{H_i})]$$
$$= \psi'_{H_i}\psi''_{H_r} - \psi''_{H_i}\psi'_{H_r}$$

Finally

$$|\psi_H|^2 = |\psi'_H|^2 + |\psi''_H|^2 + 2[\psi'_{H_i}\psi''_{H_r} - \psi'_{H_r}\psi''_{H_i}].$$

Equations 3.179 and 3.180

The assumption of equality of the three expressions 3.177 is purely a matter of convenience. However it is clear also that for crystals without centrosymmetry the calculation would become quite involved. From now on we assume that the Fourier components ψ'_H and ψ''_H are real, and for each set of Miller indices we set

$$\kappa \equiv \frac{\psi''_H}{\psi'_H},$$

where in general ψ''_H is much less than ψ'_H (due to the small anomalous part of polarizability). Equations 3.180 follow from equations 3.177:

$$|\psi_H|^2 = |\psi_{\overline{H}}|^2 \approx |\psi'_H|^2.$$

Equations 3.181

The definitions 3.181 follow the same pattern as equation 3.141. One difference is in the factor ψ_0, which is now explicitly written out as

$$\psi_0 = \psi'_0 + i\psi''_0.$$

The factor $|\psi_H|$ in the denominator is now rewritten as $|\psi'_H|$. The expression for y in equation 3.141 is now replaced by two expressions: y as before and g (absorption term).

Equation 3.182

To obtain $\sqrt{q + z^2}$ (equation 3.182), we substitute q and z^2 from equation 3.123. Equations 3.180 should be used in evaluating q, and equations 3.181 should be used in evaluating z^2.

Derivation of Equation 3.183

Within equation 3.182

$$\sqrt{1 + 2i\kappa + y^2} \;=\; \sqrt{(1 + y^2)\left(1 + \frac{2i\kappa}{1 + y^2}\right)} \;\approx\; \sqrt{(1 + y^2}\left(1 + \frac{i\kappa}{1 + y^2}\right)$$

Therefore the real part is $\sqrt{1 + y^2}$, and the imaginary part is $i\kappa/\sqrt{1 + y^2}$. This in equation 3.182 gives, using the third definition 3.181,

$$av \;=\; aK|\psi_H'|\sqrt{|b|}\,\mathrm{Re}\left[\sqrt{1 + y^2}\left(1 + \frac{i\kappa}{1 + y^2}\right)\right] \;=\; A\sqrt{1 + y^2}$$

and

$$aw \;=\; \frac{\kappa A}{\sqrt{1 + y^2}} \;.$$

Also, ignoring κ, we have

$$|q + z^2| \;=\; |v^2 + w^2| \;\approx\; K^2|\psi_H'|^2(1 + y^2).$$

Comments Following Equation 3.184

$|\psi_H'|$ is the factor appearing in A; ψ_H'' and ψ_0'' appear in the absorption term. If $\psi_0'' \ll \psi_H'$, then

$$\frac{\mu_0 t_0}{\gamma_0} \;\ll\; A.$$

Equation 3.185 is the approximation for large A, and equation 3.186 is that for small $A(<0.4)$. Equation 3.186 is readily integrated whereas one must resort to more elaborate numerical techniques in calculating R_H^y for larger κA.

Derivation of Equation 3.188

We first write by definition

$$2\kappa A \;=\; 2\frac{\psi_H''}{\psi_H'}aK|\psi_H'| \;=\; 2|\psi_H''|\frac{\pi k_0 t_0}{\gamma_0}K\frac{|\psi_0''|}{|\psi_0''|}$$

$$=\; 2\pi k_0\psi_0''\frac{t_0}{\gamma_0}\frac{|\psi_H''|}{|\psi_0''|} \;=\; \frac{\mu_0 t_0}{\gamma_0}\frac{|\psi_H''|}{|\psi_0''|} \;=\; \frac{\mu_0 t_0}{\gamma_0} \;.$$

With this definition equation 3.185 becomes

$$\frac{1}{2(1+y^2)}e^{-\mu_0 t_0/\gamma_0}\left(1 + 2\sinh^2\frac{\kappa A}{\sqrt{1+y^2}}\right) \approx \frac{1}{4(1+y^2)}e^{-\mu_0 t_0/\gamma_0[1-(\varepsilon/\sqrt{1+y^2})]}$$

To see this, we write

$$\sinh^2\frac{\kappa A}{\sqrt{1+y^2}} \equiv \sinh^2 x = \frac{(e^x - e^{-x})^2}{2} = \frac{e^{2x} + e^{-2x} - 1}{4} .$$

If we set $x = 3$, then $e^{2x} = e^6 \approx 400$ and $e^{-2x} = 0.0025$ and can be neglected; hence we have

$$\sinh^2\frac{\kappa A}{\sqrt{1+y^2}} \approx \frac{1}{4}e^{2\kappa A/\sqrt{1+y^2}}, \qquad \text{for } x > 3,$$

to one part in 400. Thus equation 3.188 follows.

Page 140: Top Two Lines

To evaluate the half-width ω_y, we proceed as previously, by setting the maximum value of equation 3.188 equal to twice the value at $\omega_y = y$:

$$\frac{1}{4(1+y^2)}e^{-(\mu_0 t_0/\gamma_0)[1-(\varepsilon/\sqrt{1+y^2})]} = \frac{1}{2}\frac{1}{4}e^{-(\mu_0 t_0/\gamma_0)(1-\varepsilon)}.$$

Taking logarithms of both sides, we obtain

$$-\log(1+y^2) + \log 2 + \frac{\mu_0 \varepsilon_0 t_0}{\gamma_0 \sqrt{1+y^2}} - \frac{\mu_0 t_0}{\gamma_0} = -\frac{\mu_0 t_0}{\gamma_0} + \frac{\mu_0 t_0}{\gamma_0}\varepsilon .$$

This equation, after simplification, is seen to be satisfied for y between 0 and 1. In fact when $2\kappa A = \mu_0 t_0/\gamma_0$ is very large, the equation holds for y very near zero. It is then reasonable to assume that

$$\log(1+y^2) \approx y^2 + \left(-\frac{y^4}{2}\right)$$

by expansion around $y = 0$. Then we have

$$-y^2 + \log 2 + \frac{2\kappa A}{\sqrt{1+y^2}} \approx 2\kappa A.$$

We now expand

$$\frac{1}{\sqrt{1+y^2}} \approx \frac{1}{1 + \frac{1}{2}y^2} \approx 1 - \frac{1}{2}y^2.$$

Hence

$$-y^2 + \log 2 + 2\kappa A \left(1 - \frac{y^2}{2}\right) \approx 2\kappa A$$

or

$$y^2 (1 + \kappa A) = +\log 2$$

or

$$y^2 = \frac{\log 2}{\kappa A + 1} \cdot$$

Thus

$$w_y = \sqrt{\frac{\log 2}{|\kappa| A + 1}} \cdot$$

The next statement that "as $|\kappa| A$ decreases to zero, w_y increases to 1," obviously does not come from the expression just derived, because the latter refers only to an approximation for large $|\kappa| A$. It may be seen from equation 3.186 that the half-width at $|\kappa| A = 0$ is equal to 1.

Page 140: Bragg Case

The Bragg case is again more difficult than the Laue case. For very thick crystals we may set sinh $aw \sim \cosh aw$ so that equation 3.139 reduces to equation 3.189. (Note that sin av then oscillates between –1 and +1 and may be ignored.)

Derivation of Equation 3.190

From equation 3.182 we get

$$|q + z^2| = K^2 |\psi'_H|^2 |b| |-(2i\kappa + 1) + y^2 + 2igy - g^2|,$$

where the minus sign is used for b in the Bragg case. From equations 3.123 and 3.180

$$q^2 = |b|^2 |\psi_H \psi_{\overline{H}}|^2 = b^2 |\psi'_H|^2 K^2 |1 + 2i\kappa|$$

$$= |b^2| |\psi'_H|^2 K^2 (1 + 4\kappa^2).$$

Substituting this in equation 3.189 namely,

$$\frac{1}{b} \frac{I_H}{I_0^e} = \frac{P_H}{P_0^e} = \frac{b|\psi_H|^2 K^2}{|q + z^2| + |z^2| + \sqrt{(|q + z^2| + |z^2|)^2 - |q|^2}} \, ,$$

we get

$$\frac{P_H}{P_0^e} = \frac{1}{L + \sqrt{L^2 - (1 + 4\kappa^2)}} \ ,$$

where we have set

$$\frac{|q + z^2| + |z^2|}{K^2 |\psi_H'|^2 |b|} \equiv L,$$

which is the same as the definition for L given by equation 3.190a, because

$$|q + z^2| = K^2 |\psi_H'|^2 |b| \sqrt{(-1 + y^2 - g^2)^2 + 4(yg - \kappa)^2}$$

$$z^2 = y^2 + g^2.$$

Then

$$\frac{P_H}{P_0} = \frac{L - \sqrt{L^2 - (1 - 4\kappa^2)}}{L^2 - (L^2 - 1 - 4\kappa^2)} = \frac{L - \sqrt{L^2 - (1 + 4\kappa^2)}}{1 + 4\kappa^2} \ .$$

Here we multiplied both the numerator and the denominator by $L - \sqrt{L^2 - (1 + 4\kappa^2)}$. Since $4\kappa^2 \ll 1$, we ignore it in the denominator and obtain equation 3.190.

Page 141: The Darwin Solution

The assumptions of the Darwin solution are stated in the subsection beginning on page 141. Here $M \equiv L$ if $g = 0$ and $\kappa = 0$, or from equation 3.190a

$$M \equiv |y^2 - 1| + y^2.$$

Equations 3.192 and 3.193

When $|y| < 1$, equation 3.192a is obvious, because $M = 1$. When $|y| \geqslant 1$, we write $M = 2y^2 - 1$, so that from equation 3.191 the expression for P_H/P_0 is

$$2y^2 - 1 - \sqrt{(2y^2 - 1)^2 - 1} = 2y^2 - 1 - \sqrt{4y^4 - 4y^2}$$

$$= 2y^2 - 1 - 2|y|\sqrt{y^2 - 1}$$

$$= (|y| - \sqrt{y^2 - 1})^2.$$

In evaluating the integral R_H^y, the expression just derived is integrated in the two regions $-\infty < y - 1$ and $+1 < y < +\infty$, whereas for $|y| < 1$ the value R_H^y is clearly $= 2$.

Furthermore since in equation 3.192b the expression for P_H/P_0 is an even function of y (changing y to $-y$ does not change the value of the function), it is necessary to evaluate only

$$2 \int_{+1}^{\infty} (y - \sqrt{y^2 - 1})^2 \, dy.$$

Page 141: Last Paragraph

The lack of symmetry is apparent by changing y to $-y$.

Equation 3.194

Equation 3.194 can be shown immediately by solving for the root of $\partial L/\partial y = 0$. On the glancing angle scale we have

$$y = \frac{\left(\dfrac{1-b}{2} |\psi_0'| + \dfrac{b}{2}\alpha\right)}{\sqrt{|b|}\, K |\psi_H'|} = \frac{\kappa}{g}$$

with α as given in our note pertaining to page 124. Therefore (see equation 3.145a)

$$\theta_0 = \theta_B + \frac{\left(\dfrac{1}{2} + \dfrac{|b|}{2}\right)|\psi_0'| - \dfrac{\kappa}{g}|\psi_H'|\sqrt{|b|}\, K}{|b| \sin 2\theta_B}.$$

The quantity $|b|$ is written as an absolute value to make equation 3.194 more universal. Note that in the Bragg case

$$\frac{1-b}{2} = \frac{1+|b|}{2}.$$

Equations 3.194 and 3.145a are similar except for the κ term. The effect of this term depends on the sign of κ. Ordinarily this term would tend to bring the peak of diffraction back to the Bragg position. However the shape would still be unsymmetric unless $\kappa = 0$.

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From equation 3.190 we evaluate the intensity maximum $(P_H/P_0)_{max}$ at $y = \kappa/g$:

$$L = \left| \sqrt{\left(-1 + \frac{\kappa^2}{g^2} - g^2\right)^2} \right| + \frac{\kappa^2}{g^2} + g^2$$

$$= \left| \sqrt{\left(1 + g^2 - \frac{\kappa^2}{g^2}\right)^2} \right| + \frac{\kappa^2}{g^2} + g^2$$

$$\approx 1 + g^2 - \frac{\kappa^2}{g^2} + \frac{\kappa^2}{g^2} + g^2$$

$$= 1 + 2g^2.$$

In the transition from the second to the third equality we used the fact that $\kappa < g$ always. So

$$\frac{P_H}{P_0} = L - \sqrt{L^2 - (1 - 4\kappa^2)} = 1 + 2g^2 - 2\sqrt{g^2(g^2 + 1 - \kappa^2)}.$$

The crude approximation $R_H^y \approx (8/3)(1 - 2|g|)$ is based on the following: When $g = 0$, $R_H^y = 8/3$, so that for very small g one might be able to write for P_H/P_0 the expression just derived:

$$\frac{P_H}{P_0} = 1 + 2g^2 - 2|g|^2\sqrt{1 + g^2 - \kappa^2}$$

$$\approx 1 + 2g^2 - 2|g|\left[1 + \frac{1}{2}(g^2 - \kappa^2)\right]$$

$$\approx 1 - 2|g|$$

or

$$R_H^y \approx \frac{8}{3}(1 - 2|g|).$$

Pages 144 to 147: Diffraction Pattern for Calcite

The diffraction pattern calculation is quite tedious but straightforward. It is suggested that the reader become familiar with structure factor calculation techniques, the simplest of which can be found in Cullity [6] and Azaroff [1]. Otherwise Zachariasen's three-page explanation of results is adequate.

Page 147: Double Crystal Diffraction Patterns

In this final section of Chapter III the experimental method of verification of pervious theory is described. Again we find the explanation quite lucid and leave the derivation entirely as an additional exercise for the reader.

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13. ABSTRACT

W. H. Zachariasen's well-known 1945 book "Theory of X-Ray Diffraction in Crystals" contains many significant and original ideas pertaining to diffraction theory. However, the discussions and mathematical derivations therein lack the necessary detail which could make the text useful to readers of diverse mathematical background. The purpose of these notes is to provide additional comments and intermediate derivational steps for Chapter III of this book, "Theory of X-Ray Diffraction in Ideal Crystals," whose content has often been referenced in the published literature.

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